wwPDB EM Validation Summary Report

Aug 4, 2026 – 06:58 PM EDT

PDB ID	:	7TTT / pdb_00007ttt
EMDB ID	:	EMD-26123
Title	:	The beta-tubulin folding intermediate III
Authors	:	Zhao, Y.; Frydman, J.; Chiu, W.
Deposited on	:	2022-02-01
Resolution	:	2.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

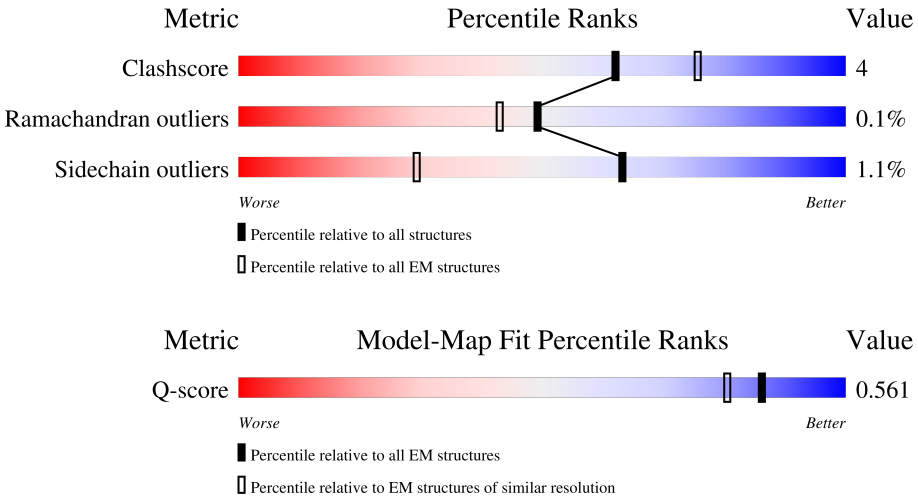
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	444	13%, 68%, 11%, 21%
2	B	547	87%, 10%
3	C	553	80%, 13%, 6%
4	D	541	86%, 11%

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Mol	Chain	Length	Quality of chain
5	E	535	
6	F	539	
7	G	556	
8	H	545	
9	I	531	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	AF3	F	603	-	-	X	-

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 35180 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	351	Total	C	N	O	S	0	0
			2750	1727	457	549	17		

- Molecule 2 is a protein called T-complex protein 1 subunit theta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	529	Total	C	N	O	S	0	0
			4029	2543	685	774	27		

- Molecule 3 is a protein called T-complex protein 1 subunit eta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	521	Total	C	N	O	S	0	0
			4003	2530	692	758	23		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	472	GLY	-	insertion	UNP Q99832
C	473	SER	-	insertion	UNP Q99832
C	474	HIS	-	insertion	UNP Q99832
C	475	HIS	-	insertion	UNP Q99832
C	476	HIS	-	insertion	UNP Q99832
C	477	HIS	-	insertion	UNP Q99832
C	478	HIS	-	insertion	UNP Q99832
C	479	HIS	-	insertion	UNP Q99832
C	480	GLY	-	insertion	UNP Q99832
C	481	SER	-	insertion	UNP Q99832

- Molecule 4 is a protein called T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	528	Total	C	N	O	S	0	0
			4072	2549	711	782	30		

- Molecule 5 is a protein called T-complex protein 1 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	526	Total	C	N	O	S	0	0
			3960	2478	699	764	19		

- Molecule 6 is a protein called T-complex protein 1 subunit delta.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	520	Total	C	N	O	S	0	0
			3924	2453	683	765	23		

- Molecule 7 is a protein called T-complex protein 1 subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	535	Total	C	N	O	S	0	0
			4063	2545	710	785	23		

- Molecule 8 is a protein called T-complex protein 1 subunit gamma.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	523	Total	C	N	O	S	0	0
			4064	2534	718	782	30		

- Molecule 9 is a protein called T-complex protein 1 subunit zeta.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	528	Total	C	N	O	S	0	0
			4051	2549	708	773	21		

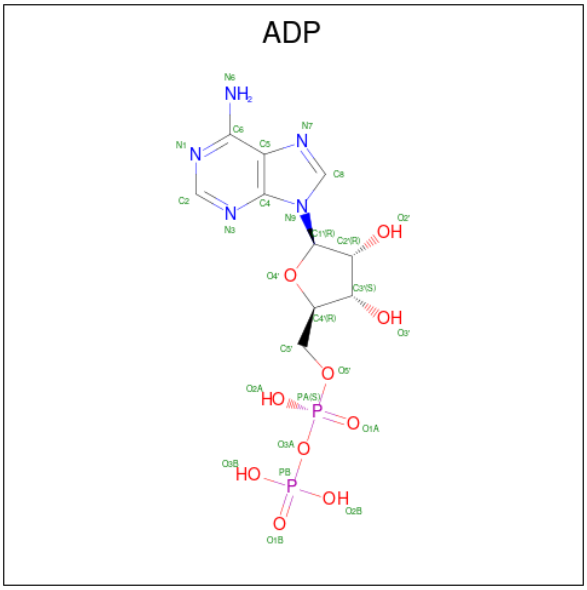
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	528	PHE	SER	conflict	UNP P40227

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
10	B	1	Total Mg 1 1	0
10	C	1	Total Mg 1 1	0
10	D	1	Total Mg 1 1	0
10	E	1	Total Mg 1 1	0
10	F	1	Total Mg 1 1	0
10	G	1	Total Mg 1 1	0
10	H	1	Total Mg 1 1	0
10	I	1	Total Mg 1 1	0

- Molecule 11 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



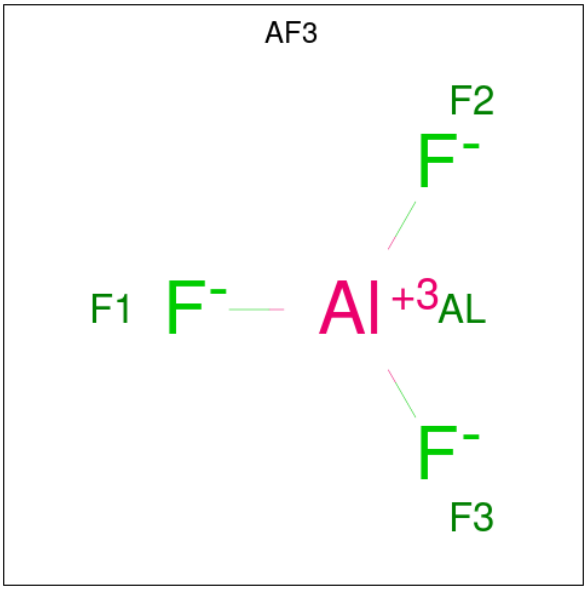
Mol	Chain	Residues	Atoms	AltConf
11	B	1	Total C N O P 27 10 5 10 2	0
11	C	1	Total C N O P 27 10 5 10 2	0
11	D	1	Total C N O P 27 10 5 10 2	0

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Mol	Chain	Residues	Atoms					AltConf
11	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
11	I	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 12 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
12	B	1	Total	Al	F	0
			4	1	3	
12	C	1	Total	Al	F	0
			4	1	3	
12	D	1	Total	Al	F	0
			4	1	3	
12	E	1	Total	Al	F	0
			4	1	3	
12	F	1	Total	Al	F	0
			4	1	3	
12	G	1	Total	Al	F	0
			4	1	3	

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Mol	Chain	Residues	Atoms	AltConf
12	H	1	Total Al F 4 1 3	0
12	I	1	Total Al F 4 1 3	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	AltConf
13	B	1	Total O 1 1	0
13	C	1	Total O 1 1	0
13	D	1	Total O 1 1	0
13	E	1	Total O 1 1	0
13	F	1	Total O 1 1	0
13	G	1	Total O 1 1	0
13	H	1	Total O 1 1	0
13	I	1	Total O 1 1	0

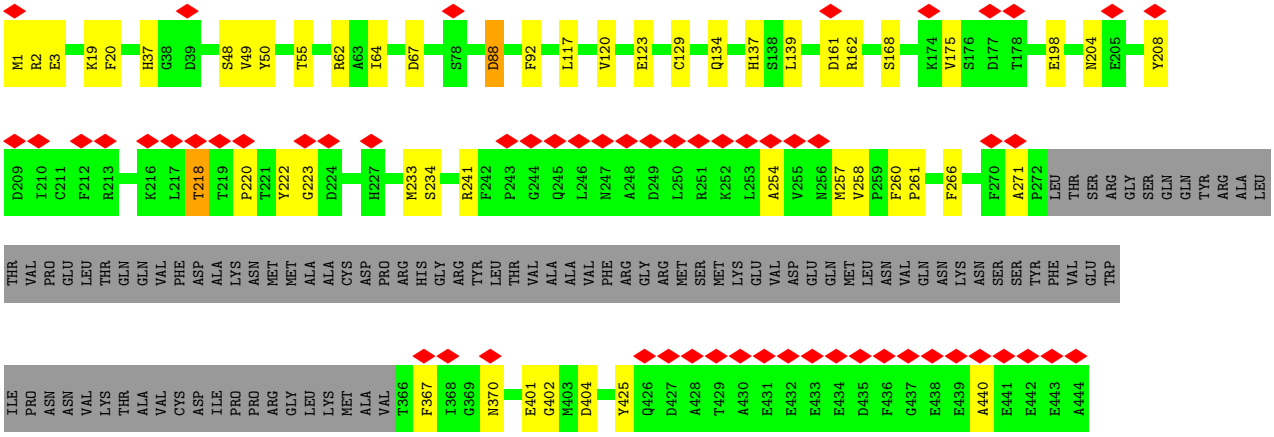
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin beta chain

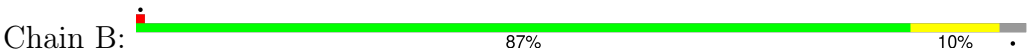
Chain A:

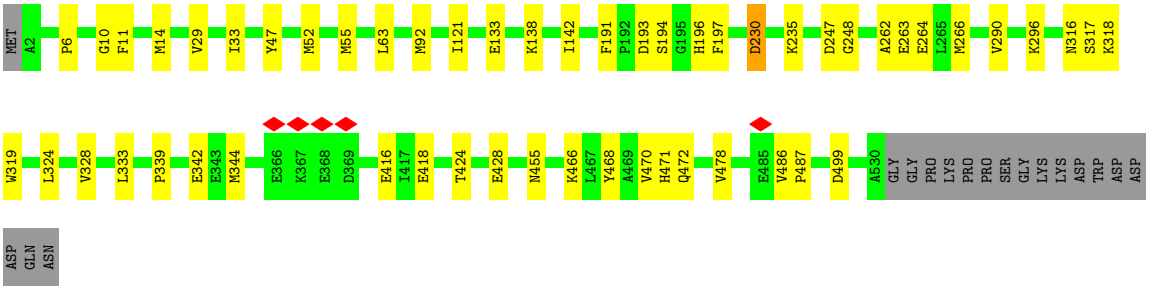




• Molecule 2: T-complex protein 1 subunit theta

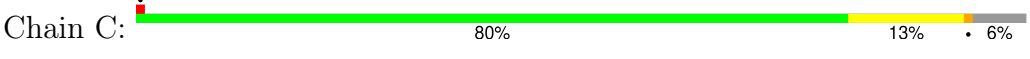
Chain B:

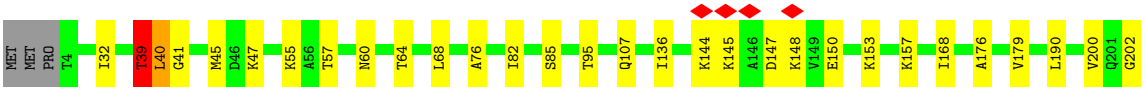


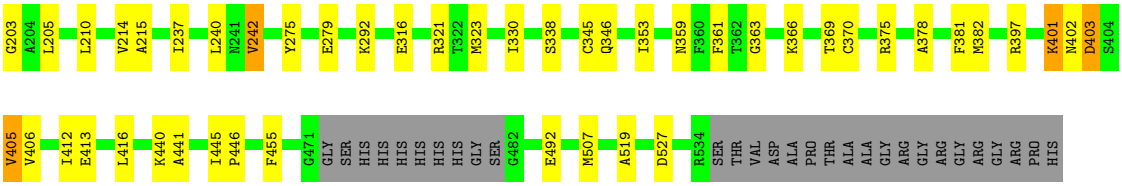


• Molecule 3: T-complex protein 1 subunit eta

Chain C:







• Molecule 4: T-complex protein 1 subunit epsilon

Chain D:

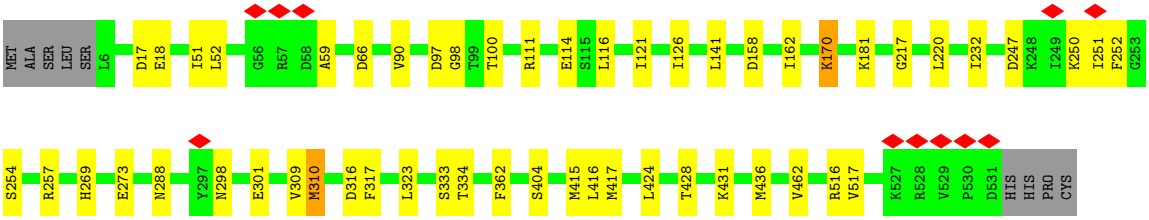




• Molecule 5: T-complex protein 1 subunit beta

Chain E:

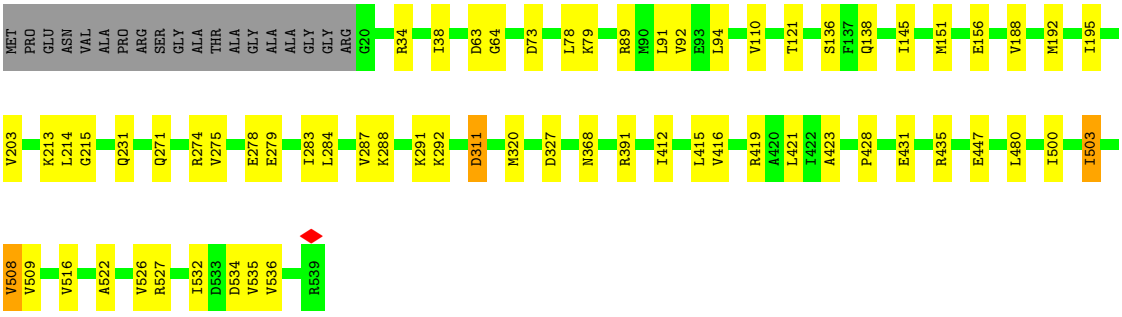




• Molecule 6: T-complex protein 1 subunit delta

Chain F:

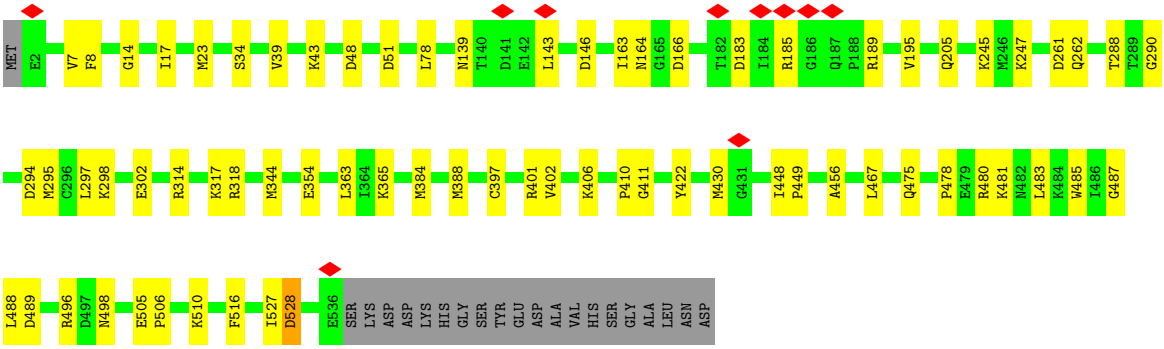




• Molecule 7: T-complex protein 1 subunit alpha

Chain G:

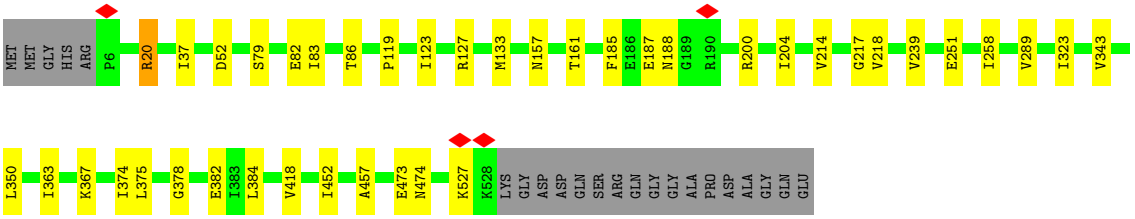




• Molecule 8: T-complex protein 1 subunit gamma

Chain H:

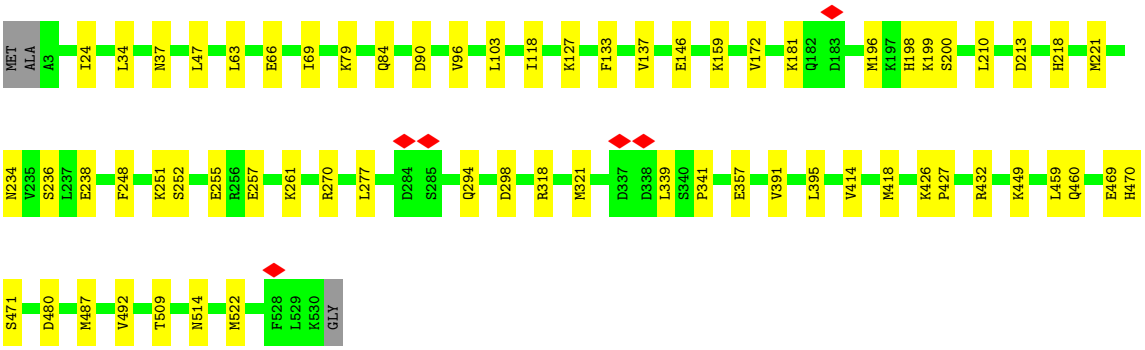




• Molecule 9: T-complex protein 1 subunit zeta

Chain I:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	94955	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.21	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	21.010	Depositor
Minimum map value	-8.335	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	3.31	Depositor
Map size (Å)	352.0, 352.0, 352.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.19	0/2811	0.46	1/3810 (0.0%)
2	B	0.28	0/4087	0.46	4/5525 (0.1%)
3	C	0.33	5/4058 (0.1%)	0.45	5/5476 (0.1%)
4	D	0.18	0/4121	0.39	0/5551
5	E	0.28	3/4004 (0.1%)	0.40	0/5399
6	F	0.17	0/3956	0.35	0/5338
7	G	0.22	1/4103 (0.0%)	0.40	1/5540 (0.0%)
8	H	0.18	0/4110	0.38	0/5544
9	I	0.22	1/4099 (0.0%)	0.39	0/5525
All	All	0.23	10/35349 (0.0%)	0.41	11/47708 (0.0%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	40	LEU	C-O	-7.14	1.15	1.24
5	E	100	THR	C-O	-6.98	1.15	1.24
3	C	405	VAL	C-O	-6.23	1.17	1.24
5	E	98	GLY	C-O	-6.09	1.16	1.24
3	C	406	VAL	C-O	-6.05	1.16	1.23

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	528	ASP	CA-CB-CG	6.61	119.21	112.60
2	B	191	PHE	CA-CB-CG	6.20	120.00	113.80
3	C	41	GLY	CA-C-N	6.09	125.71	119.56
3	C	41	GLY	C-N-CA	6.09	125.71	119.56
2	B	230	ASP	CA-CB-CG	5.87	118.47	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2750	0	2599	32	0
2	B	4029	0	4099	29	0
3	C	4003	0	4106	43	0
4	D	4072	0	4189	39	0
5	E	3960	0	4077	29	0
6	F	3924	0	4131	41	0
7	G	4063	0	4219	46	0
8	H	4064	0	4202	29	0
9	I	4051	0	4194	40	0
10	B	1	0	0	0	0
10	C	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0
10	H	1	0	0	0	0
10	I	1	0	0	0	0
11	B	27	0	12	0	0
11	C	27	0	12	0	0
11	D	27	0	12	1	0
11	E	27	0	12	0	0
11	F	27	0	12	0	0
11	G	27	0	12	1	0
11	H	27	0	12	0	0
11	I	27	0	12	0	0
12	B	4	0	0	0	0
12	C	4	0	0	1	0
12	D	4	0	0	1	0
12	E	4	0	0	1	0
12	F	4	0	0	2	0
12	G	4	0	0	1	0
12	H	4	0	0	0	0
12	I	4	0	0	1	0
13	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C	1	0	0	0	0
13	D	1	0	0	0	0
13	E	1	0	0	0	0
13	F	1	0	0	0	0
13	G	1	0	0	0	0
13	H	1	0	0	0	0
13	I	1	0	0	0	0
All	All	35180	0	35912	304	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 304 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:ASP:HA	12:E:603:AF3:F3	1.60	0.92
6:F:73:ASP:HA	12:F:603:AF3:F3	1.63	0.88
9:I:414:VAL:HG22	9:I:418:MET:HE2	1.66	0.76
1:A:440:ALA:HA	7:G:189:ARG:HH12	1.52	0.75
4:D:58:ASP:OD2	5:E:516:ARG:NH1	2.20	0.75

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	347/444 (78%)	328 (94%)	17 (5%)	2 (1%)	21	51
2	B	527/547 (96%)	512 (97%)	14 (3%)	1 (0%)	43	72
3	C	517/553 (94%)	498 (96%)	18 (4%)	1 (0%)	43	72
4	D	526/541 (97%)	504 (96%)	21 (4%)	1 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	524/535 (98%)	501 (96%)	23 (4%)	0	100	100
6	F	518/539 (96%)	508 (98%)	10 (2%)	0	100	100
7	G	533/556 (96%)	502 (94%)	31 (6%)	0	100	100
8	H	521/545 (96%)	501 (96%)	20 (4%)	0	100	100
9	I	526/531 (99%)	502 (95%)	23 (4%)	1 (0%)	43	72
All	All	4539/4791 (95%)	4356 (96%)	177 (4%)	6 (0%)	49	77

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	401	LYS
1	A	223	GLY
4	D	156	LEU
9	I	200	SER
1	A	271	ALA

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/379 (79%)	293 (98%)	5 (2%)	53	82
2	B	436/451 (97%)	429 (98%)	7 (2%)	55	83
3	C	428/451 (95%)	420 (98%)	8 (2%)	50	79
4	D	446/456 (98%)	444 (100%)	2 (0%)	84	94
5	E	419/427 (98%)	412 (98%)	7 (2%)	53	82
6	F	442/452 (98%)	438 (99%)	4 (1%)	70	90
7	G	446/463 (96%)	443 (99%)	3 (1%)	76	92
8	H	454/469 (97%)	453 (100%)	1 (0%)	87	96
9	I	441/442 (100%)	435 (99%)	6 (1%)	59	85
All	All	3810/3990 (96%)	3767 (99%)	43 (1%)	63	88

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	E	416	LEU
7	G	528	ASP
6	F	311	ASP
6	F	508	VAL
9	I	84	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	420	HIS
8	H	504	GLN
5	E	73	ASN
4	D	516	GLN
8	H	526	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	ADP	G	602	10,12	28,29,29	1.39	4 (14%)	43,45,45	1.84	9 (20%)
12	AF3	B	603	-	0,3,3	-	-	-		
12	AF3	H	603	8	0,3,3	-	-	-		
12	AF3	I	603	-	0,3,3	-	-	-		
11	ADP	I	602	10	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)
12	AF3	D	603	11	0,3,3	-	-	-		
12	AF3	C	603	-	0,3,3	-	-	-		
12	AF3	E	603	5	0,3,3	-	-	-		
11	ADP	H	602	10	28,29,29	1.38	4 (14%)	43,45,45	1.85	9 (20%)
11	ADP	C	602	10	28,29,29	1.37	4 (14%)	43,45,45	1.94	11 (25%)
11	ADP	E	602	10	28,29,29	1.38	4 (14%)	43,45,45	1.86	9 (20%)
11	ADP	F	602	10	28,29,29	1.37	4 (14%)	43,45,45	1.85	10 (23%)
11	ADP	D	602	10,12	28,29,29	1.39	4 (14%)	43,45,45	1.86	9 (20%)
12	AF3	F	603	-	0,3,3	-	-	-		
11	ADP	B	602	10	28,29,29	1.37	5 (17%)	43,45,45	1.89	10 (23%)
12	AF3	G	603	11	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ADP	G	602	10,12	-	1/16/32/32	0/3/3/3
11	ADP	I	602	10	-	3/16/32/32	0/3/3/3
11	ADP	H	602	10	-	5/16/32/32	0/3/3/3
11	ADP	C	602	10	-	1/16/32/32	0/3/3/3
11	ADP	E	602	10	-	6/16/32/32	0/3/3/3
11	ADP	F	602	10	-	7/16/32/32	0/3/3/3
11	ADP	D	602	10,12	-	1/16/32/32	0/3/3/3
11	ADP	B	602	10	-	6/16/32/32	0/3/3/3

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	602	ADP	C5-C4	4.51	1.47	1.39
11	E	602	ADP	C5-C4	4.50	1.47	1.39
11	H	602	ADP	C5-C4	4.47	1.47	1.39
11	G	602	ADP	C5-C4	4.46	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	602	ADP	C5-C4	4.45	1.47	1.39

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	602	ADP	C5-C4-N3	-5.95	118.52	126.72
11	E	602	ADP	C5-C4-N3	-5.93	118.55	126.72
11	I	602	ADP	C5-C4-N3	-5.93	118.56	126.72
11	C	602	ADP	C5-C4-N3	-5.92	118.57	126.72
11	D	602	ADP	C5-C4-N3	-5.90	118.59	126.72

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	D	602	ADP	PB-O3A-PA-O5'
11	E	602	ADP	C5'-O5'-PA-O1A
11	E	602	ADP	C5'-O5'-PA-O2A
11	E	602	ADP	C5'-O5'-PA-O3A
11	F	602	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

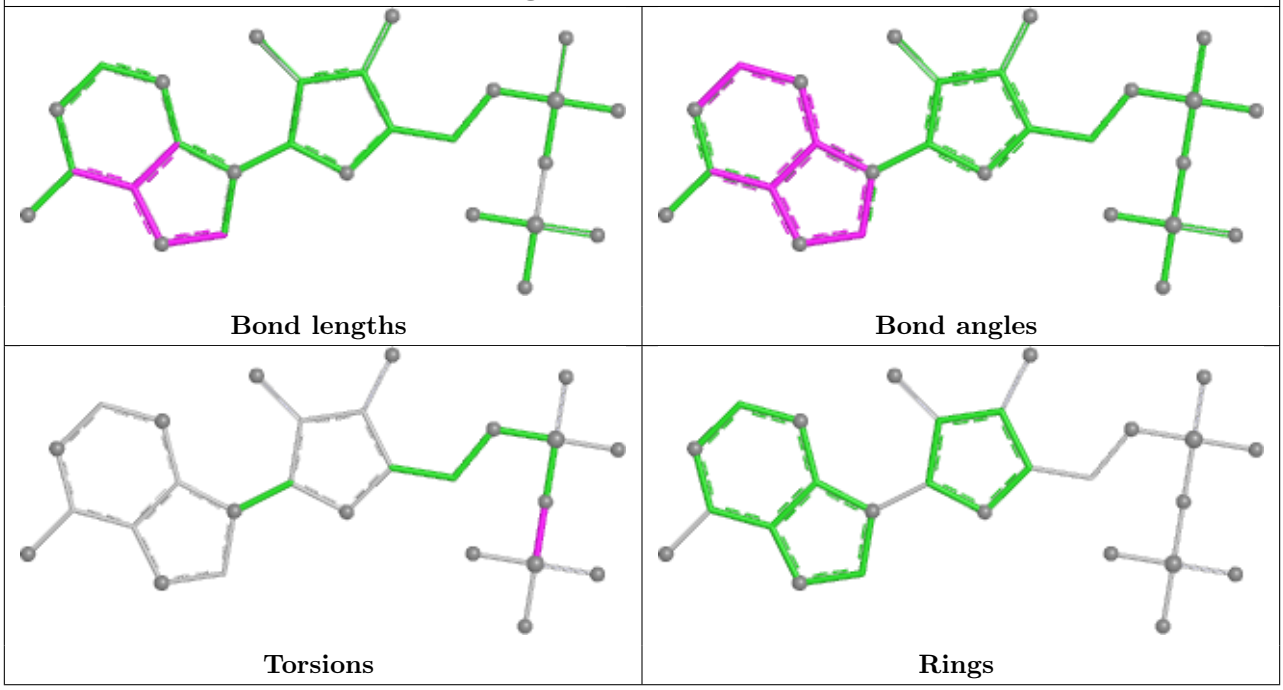
8 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	G	602	ADP	1	0
12	I	603	AF3	1	0
12	D	603	AF3	1	0
12	C	603	AF3	1	0
12	E	603	AF3	1	0
11	D	602	ADP	1	0
12	F	603	AF3	2	0
12	G	603	AF3	1	0

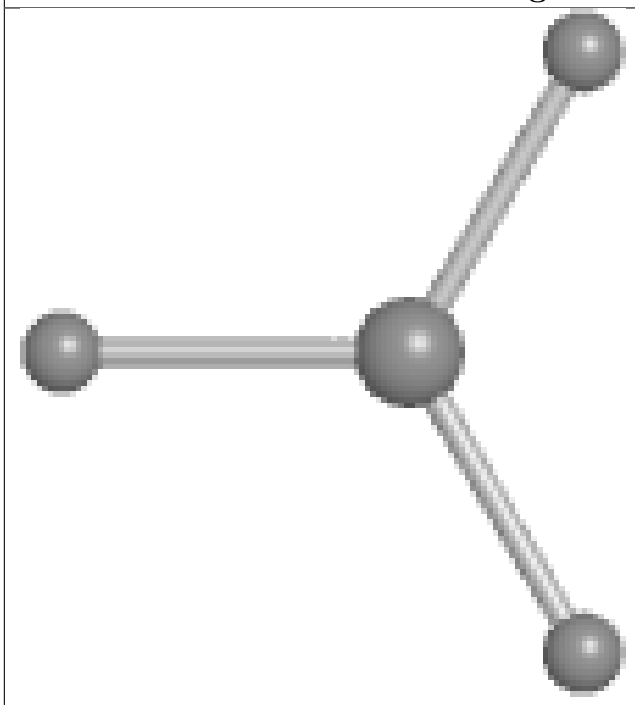
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

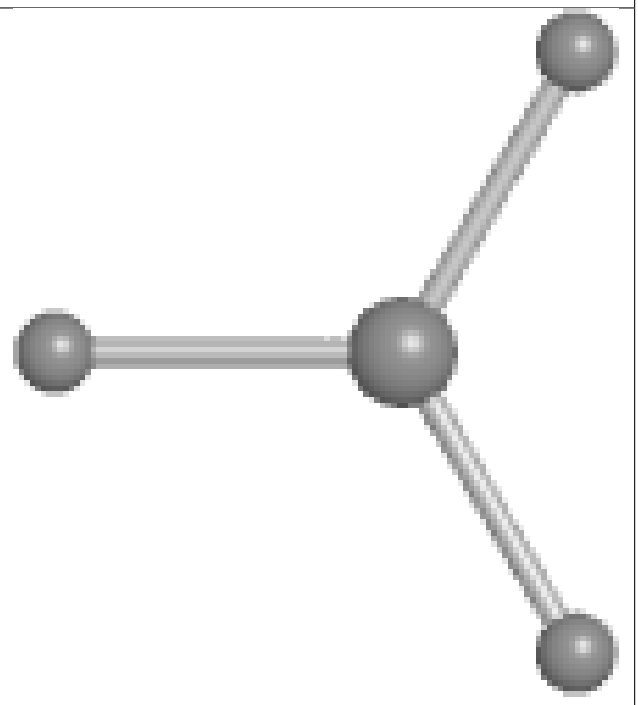
Ligand ADP G 602



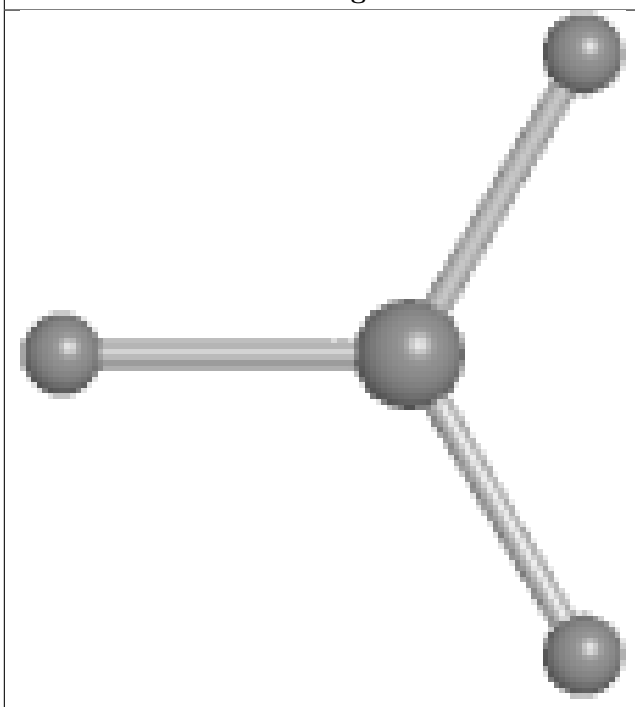
Ligand AF3 B 603



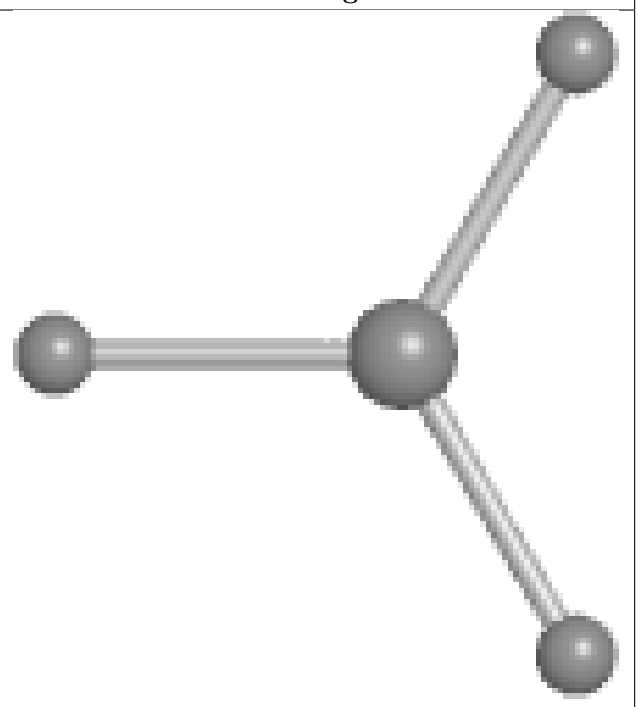
Bond lengths



Bond angles

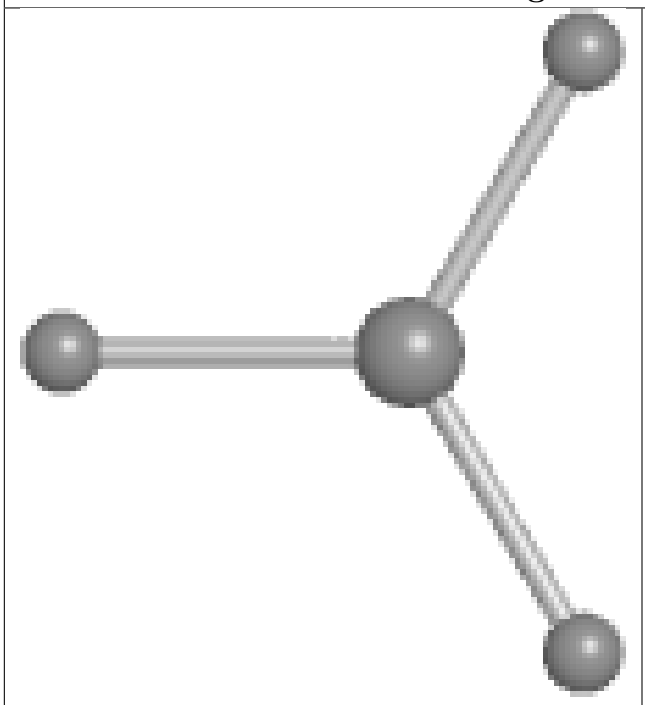


Torsions

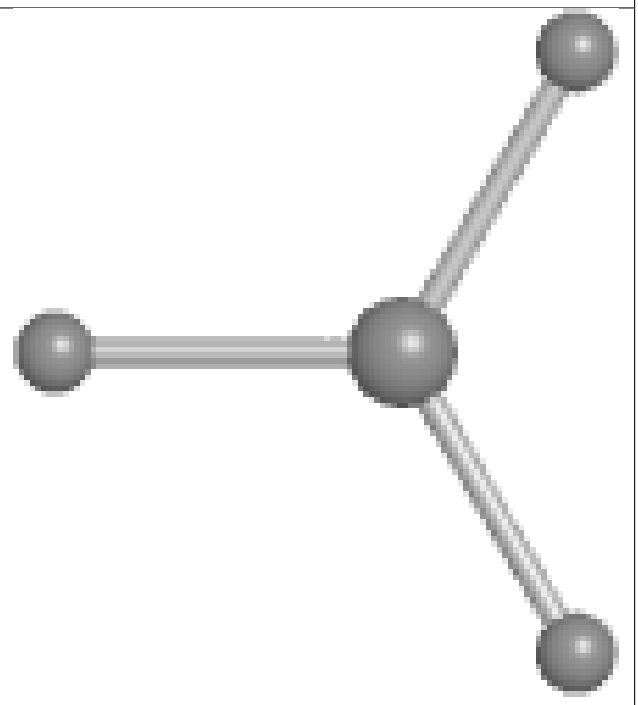


Rings

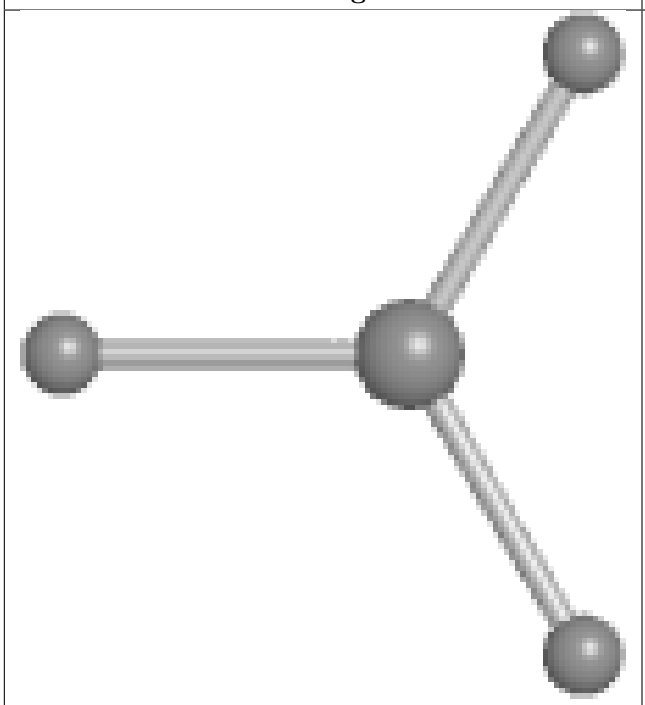
Ligand AF3 H 603



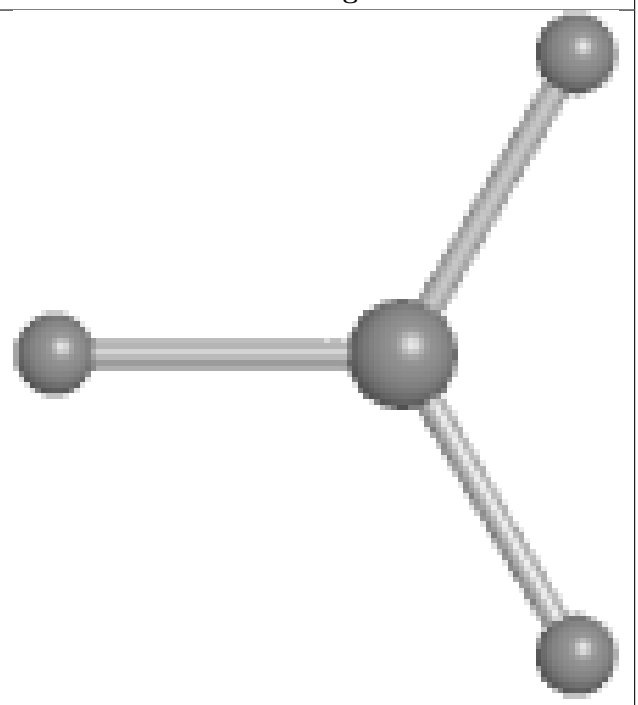
Bond lengths



Bond angles

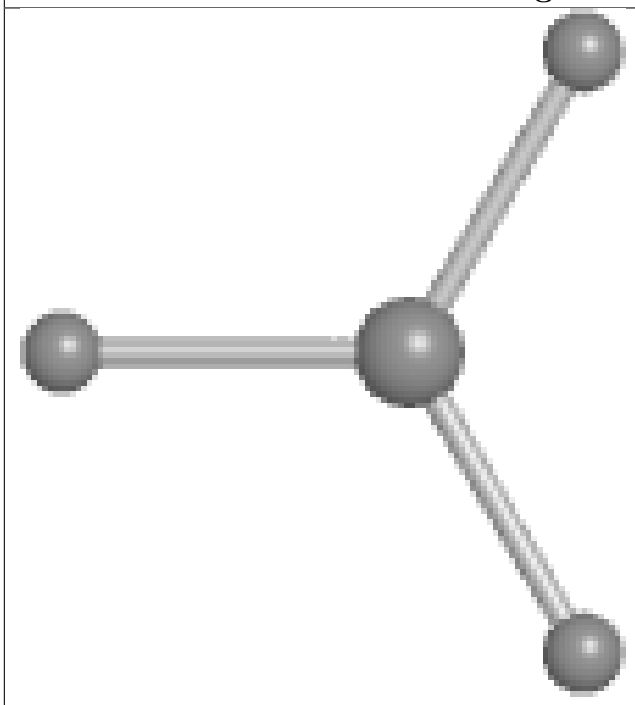


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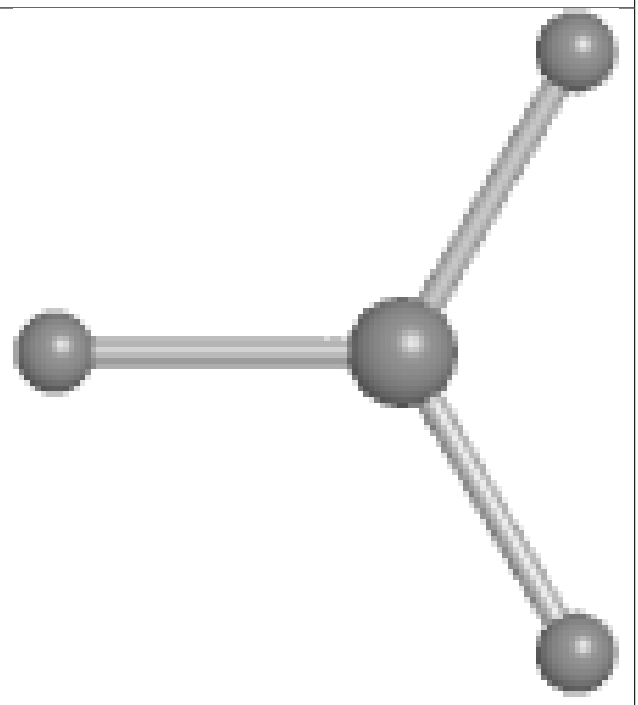


Rings

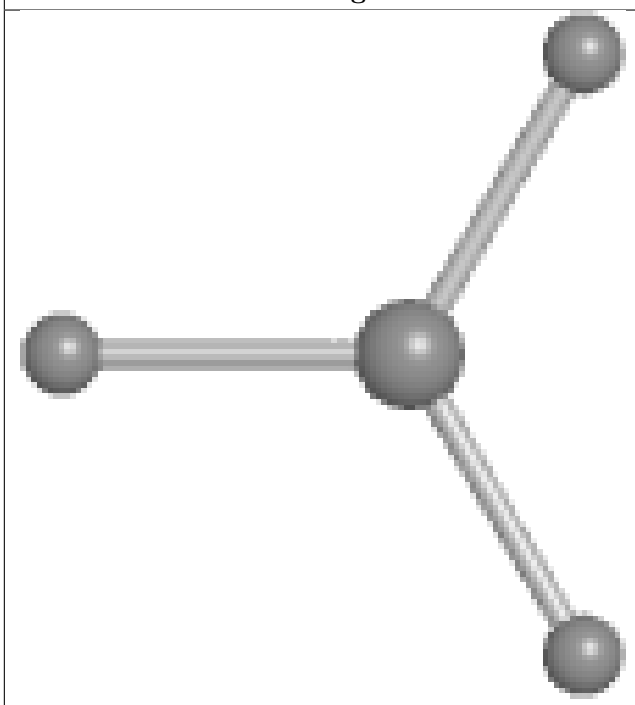
Ligand AF3 I 603



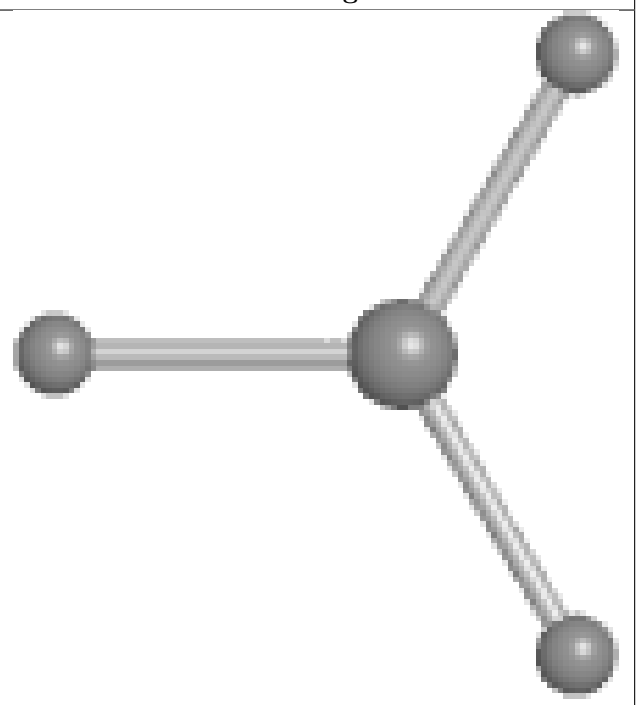
Bond lengths



Bond angles

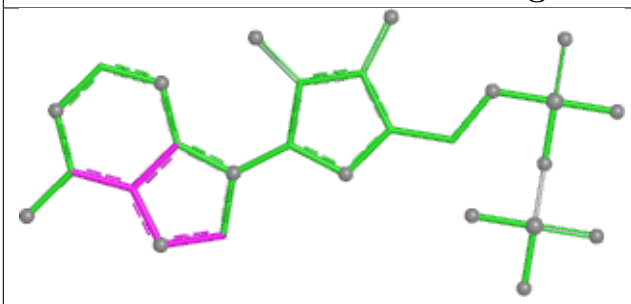


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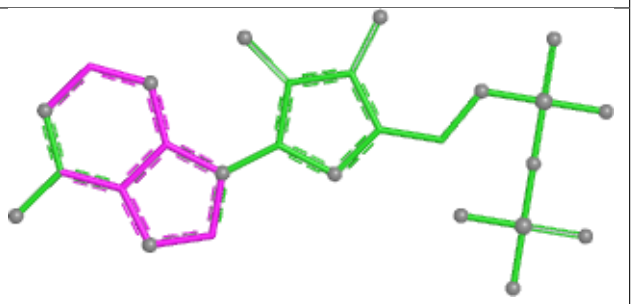


Rings

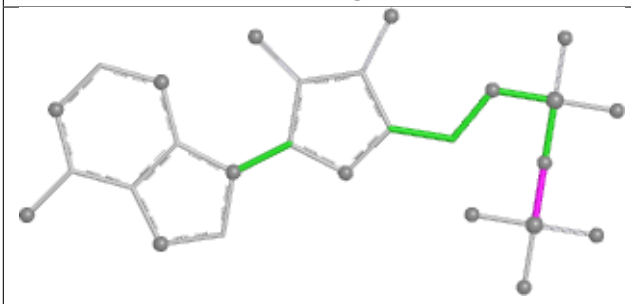
Ligand ADP I 602



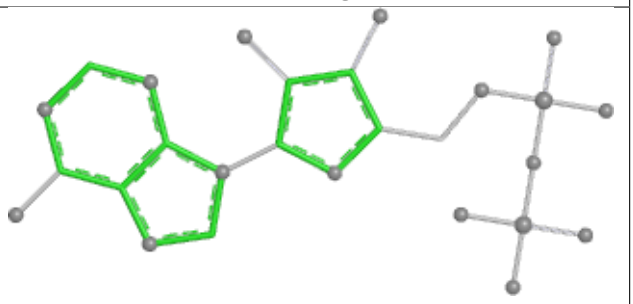
Bond lengths



Bond angles

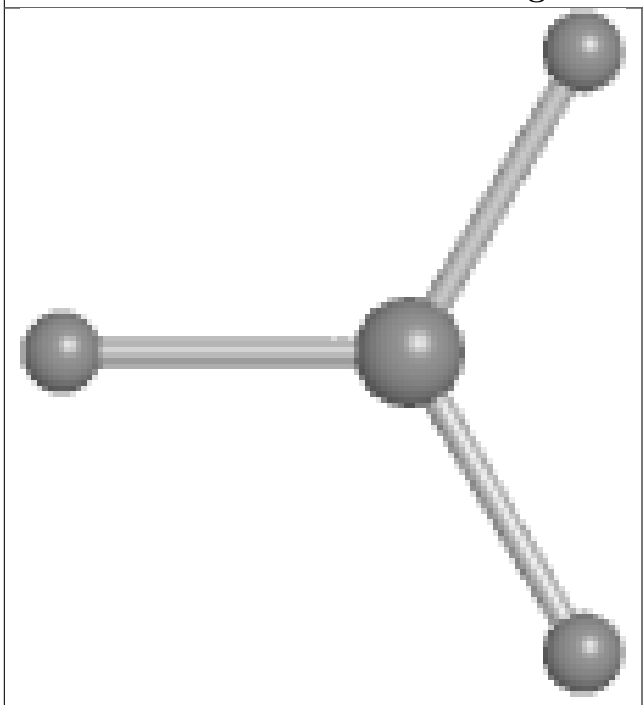


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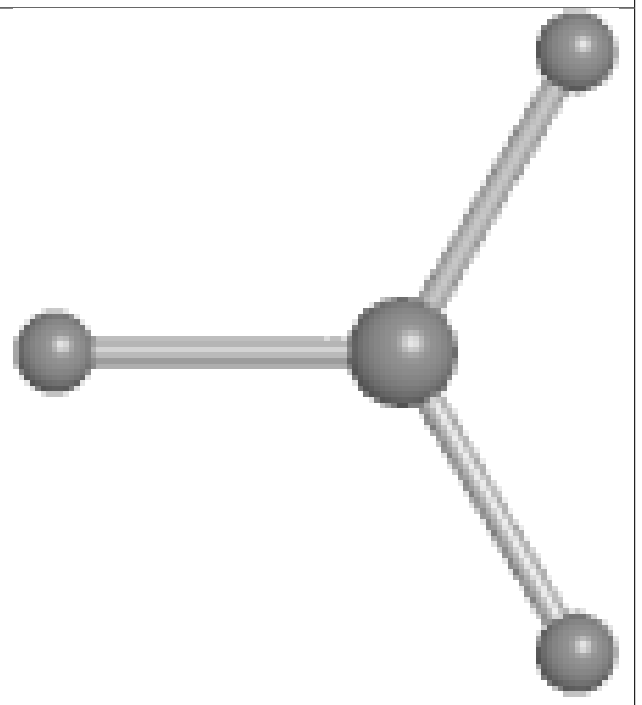


Rings

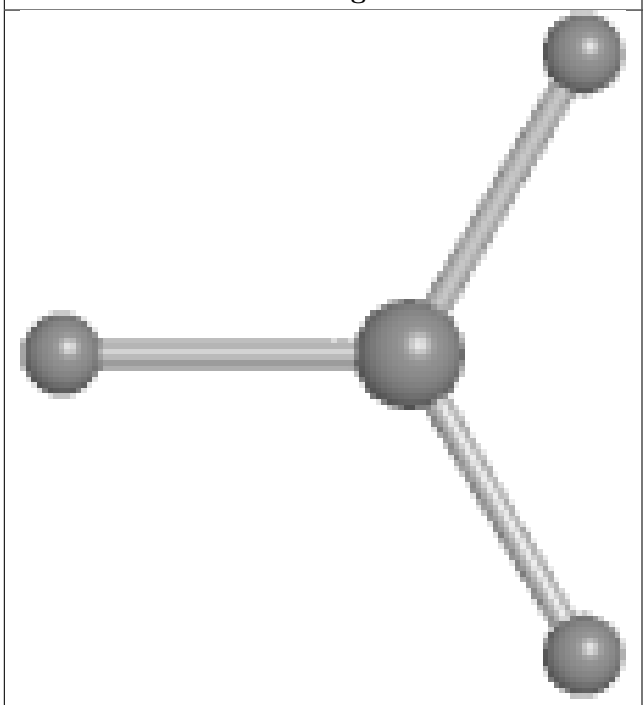
Ligand AF3 D 603



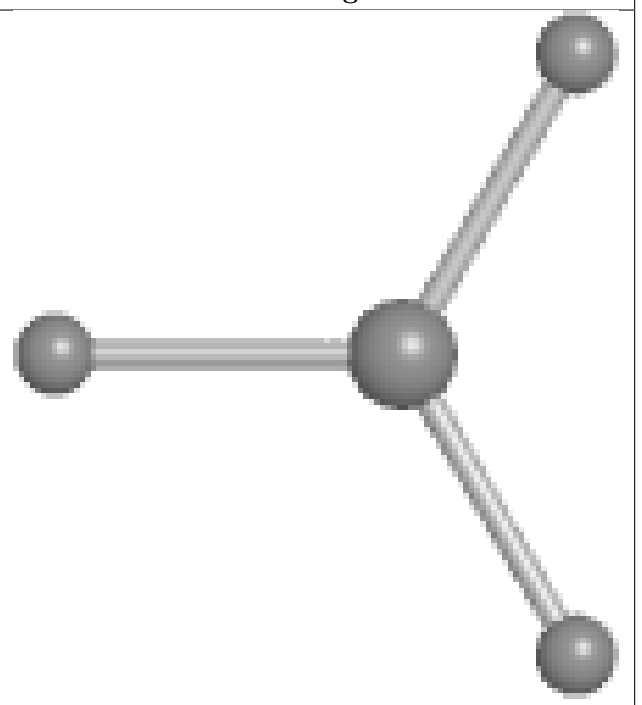
Bond lengths



Bond angles

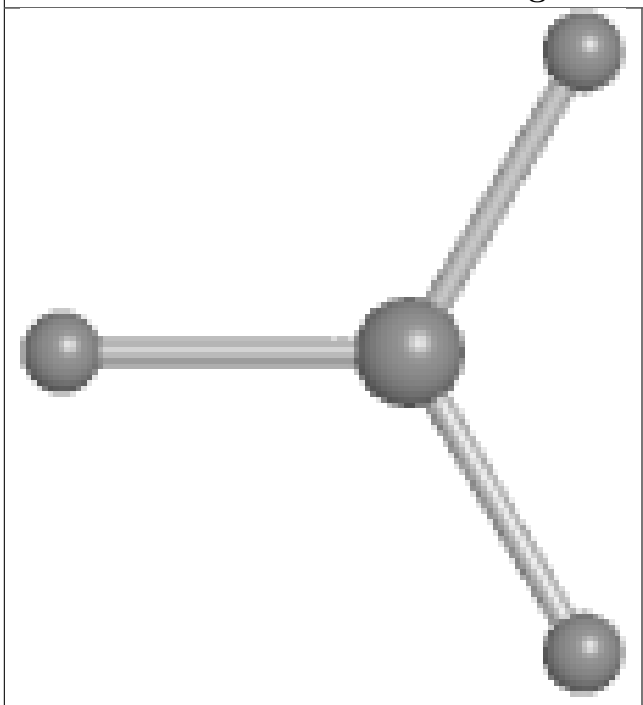


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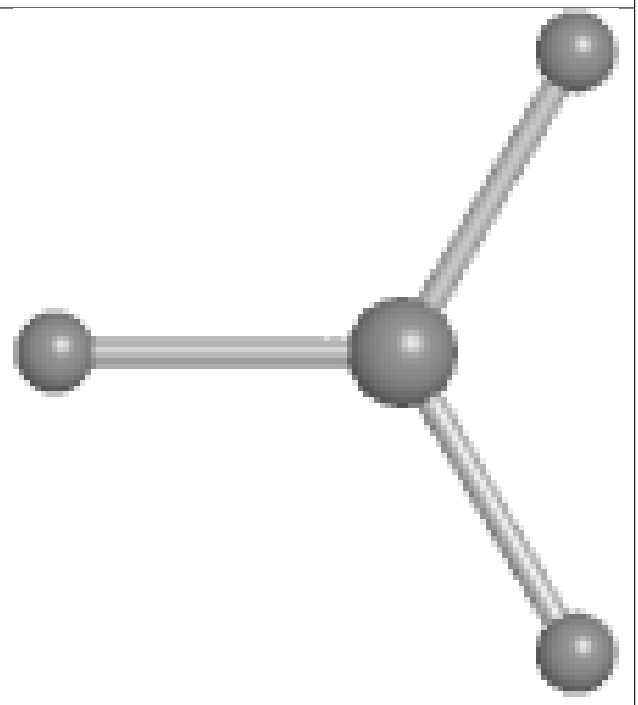


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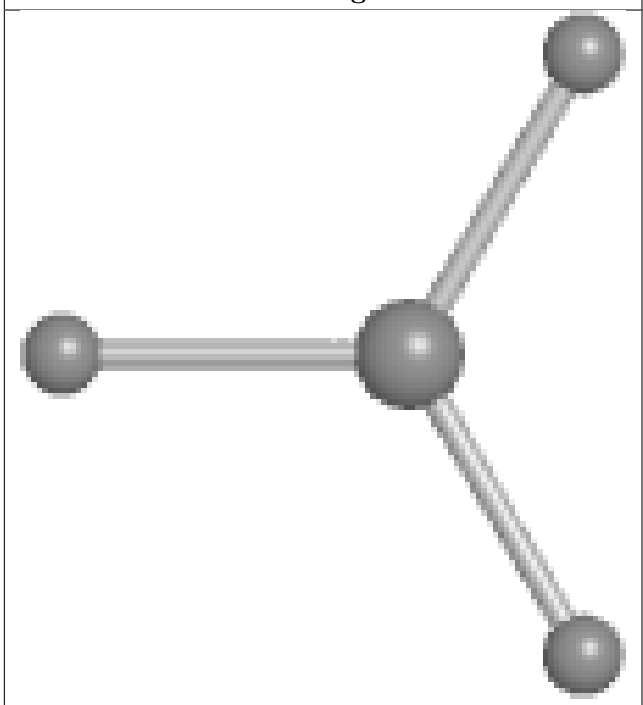
Ligand AF3 C 603



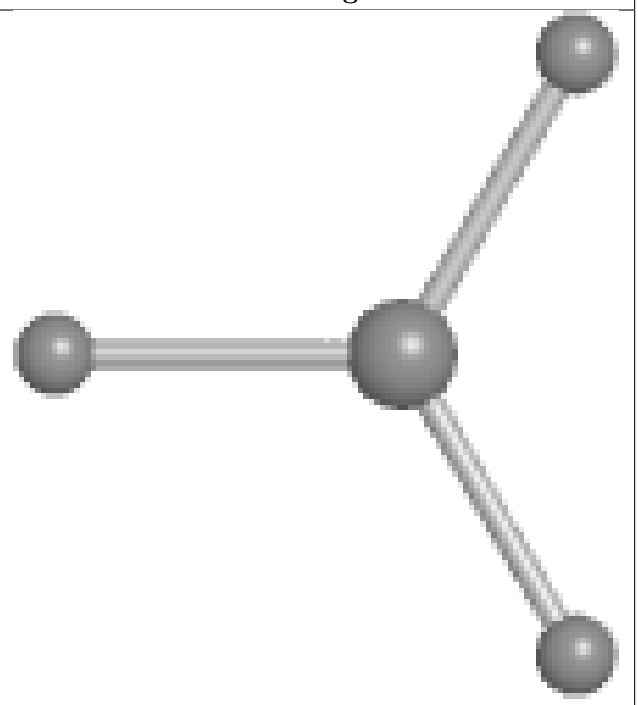
Bond lengths



Bond angles

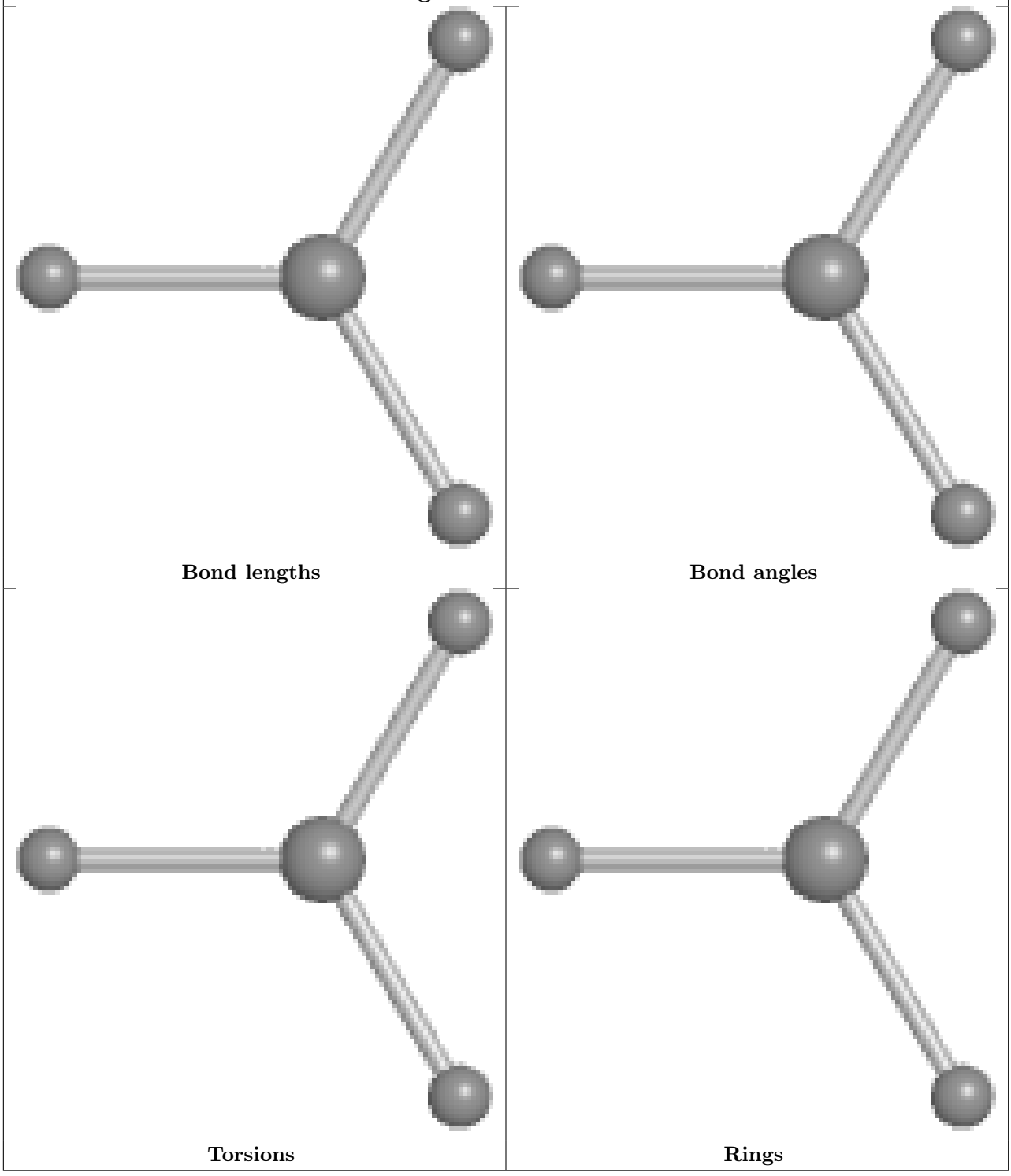


Torsions



Rings

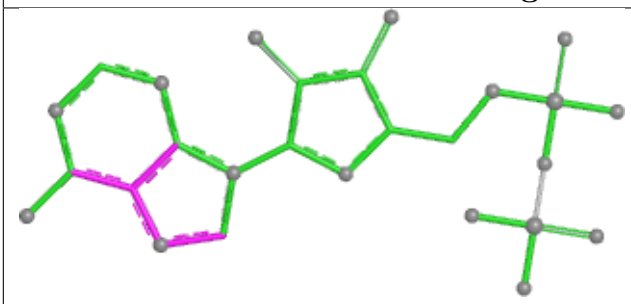
Ligand AF3 E 603



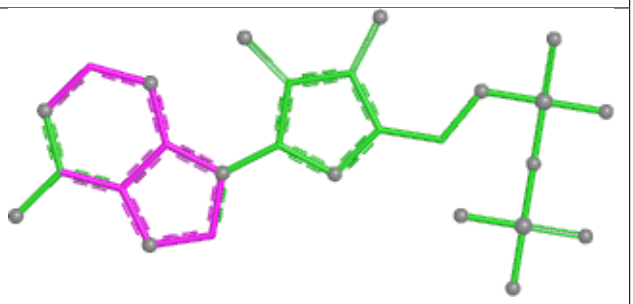
Bond lengths **Bond angles**

Torsions **Rings**

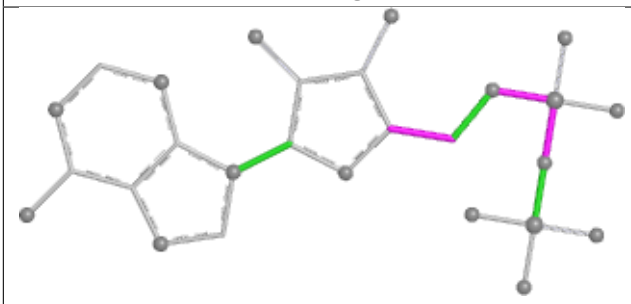
Ligand ADP H 602



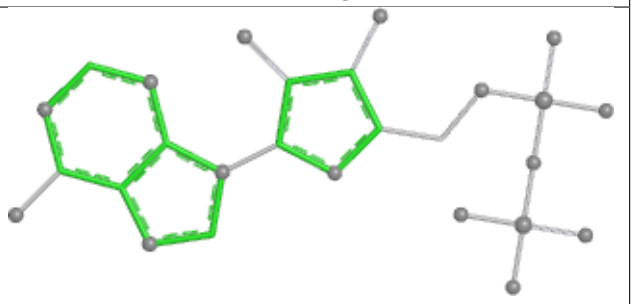
Bond lengths



Bond angles

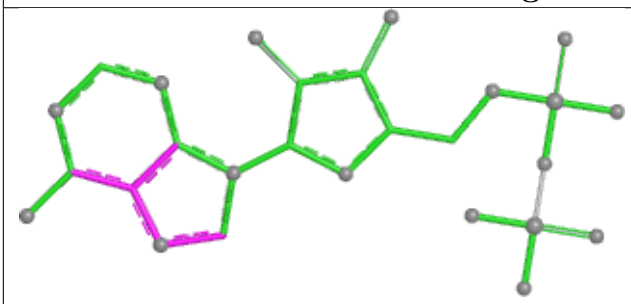


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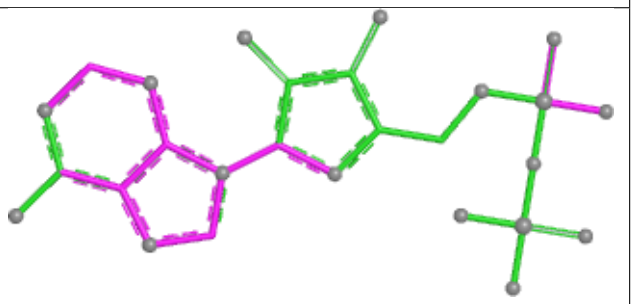


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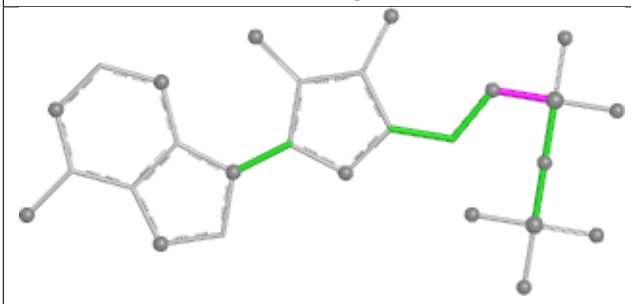
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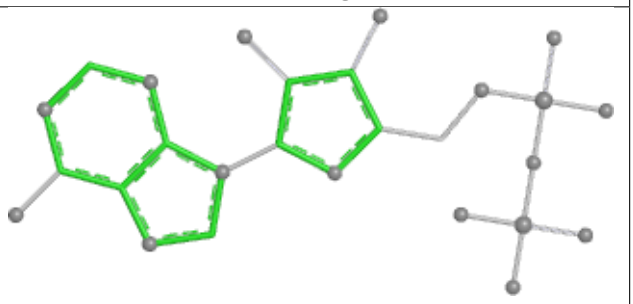
Bond lengths



Bond angles

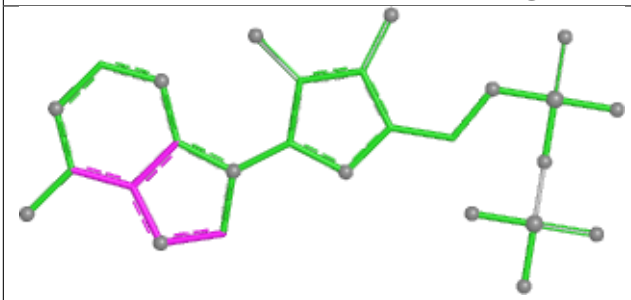


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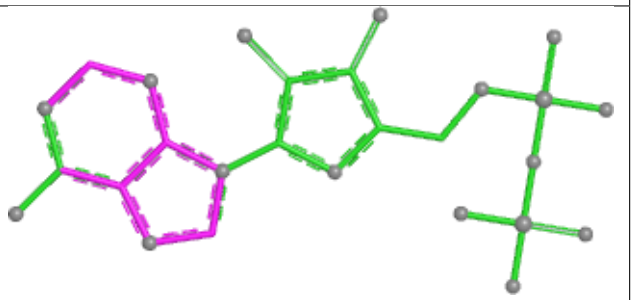


Rings

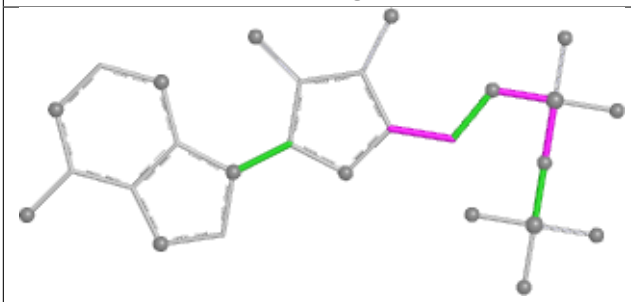
Ligand ADP E 602



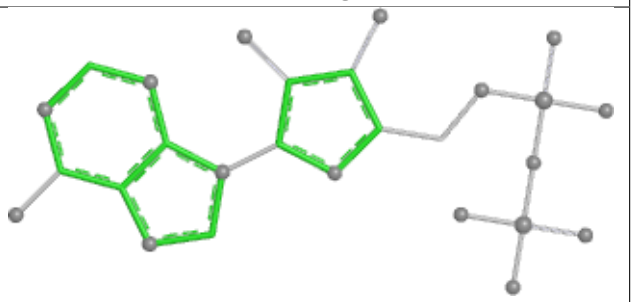
Bond lengths



Bond angles

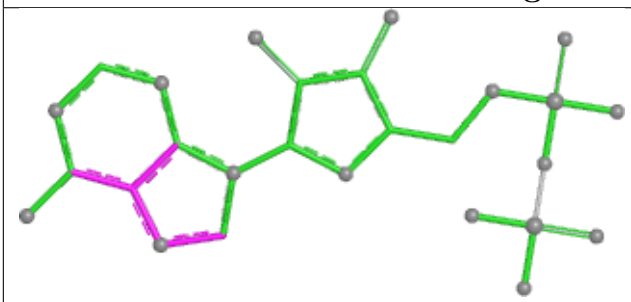


Torsions

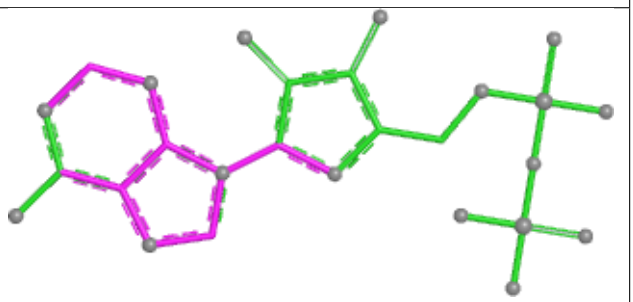


Rings

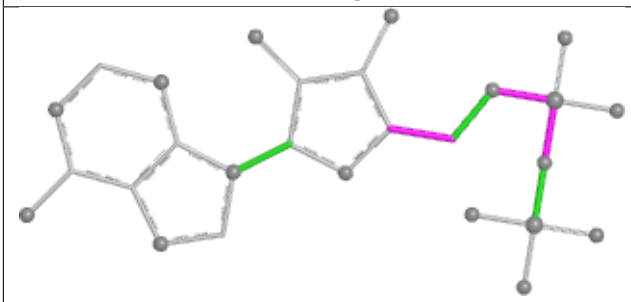
Ligand ADP F 602



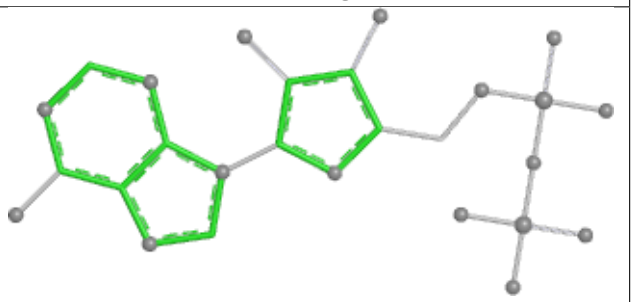
Bond lengths



Bond angles

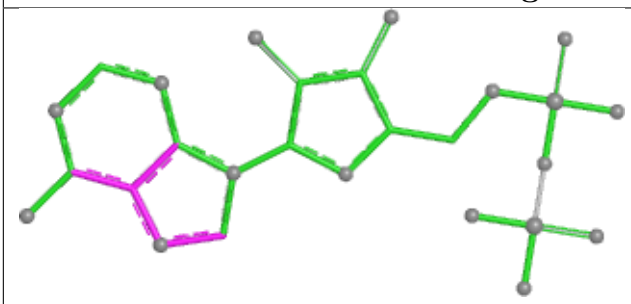


Torsions

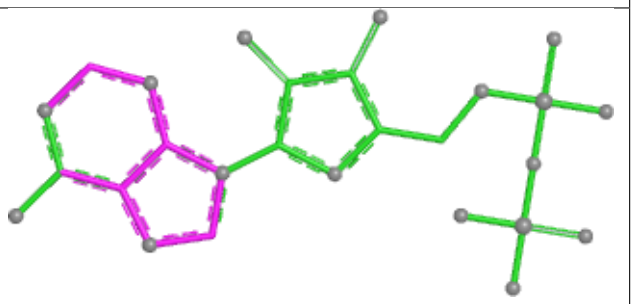


Rings

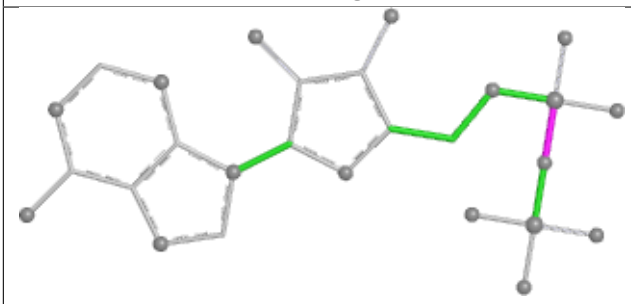
Ligand ADP D 602



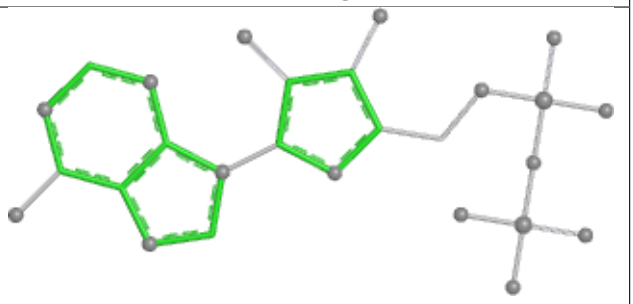
Bond lengths



Bond angles

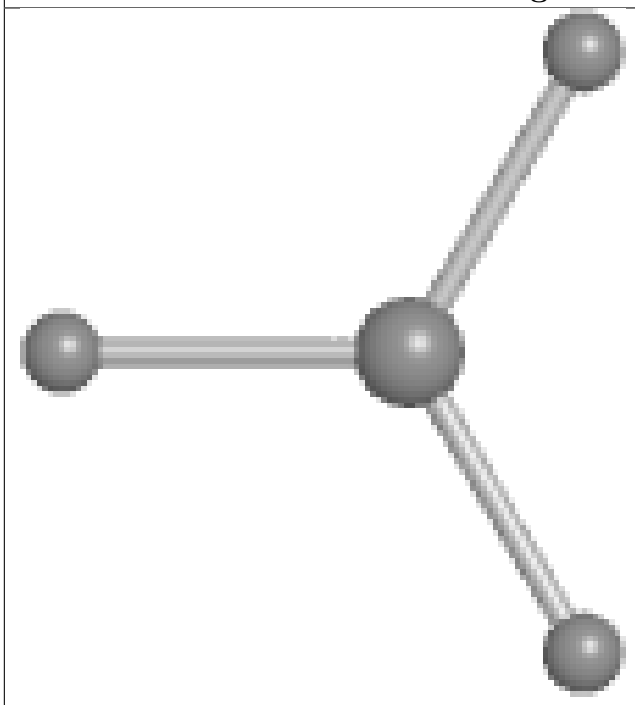


Torsions

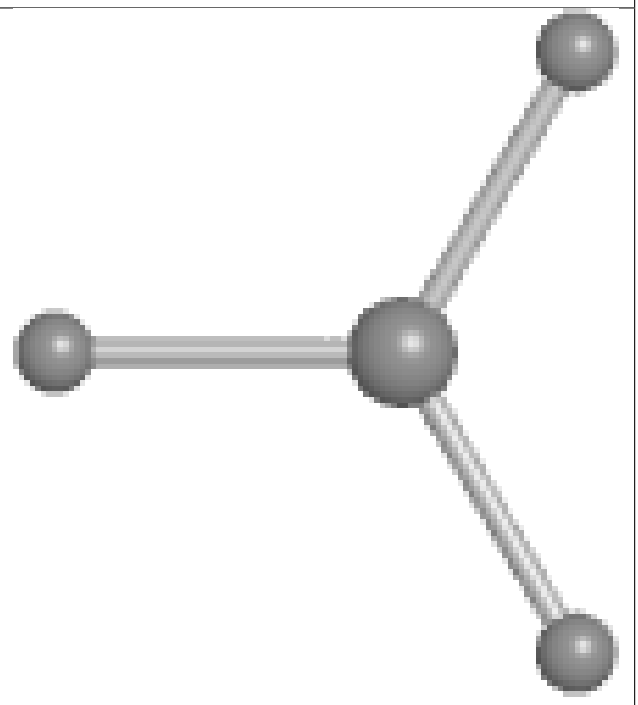


Rings

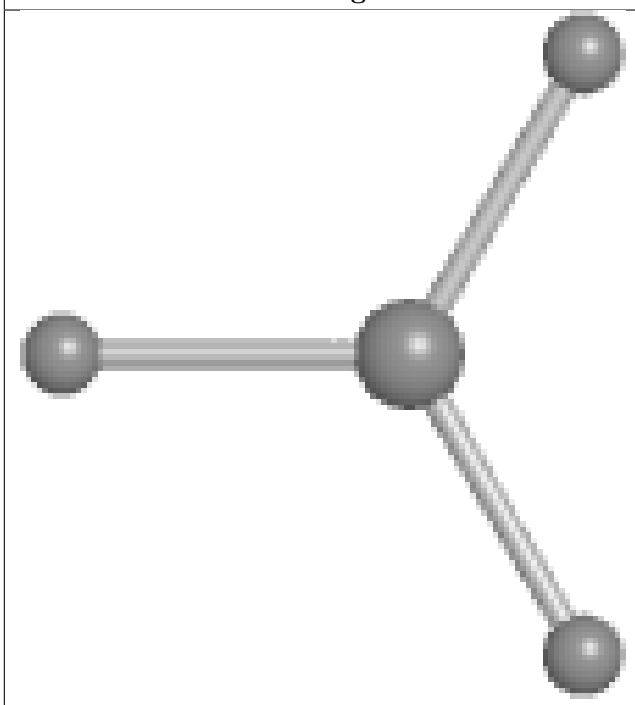
Ligand AF3 F 603



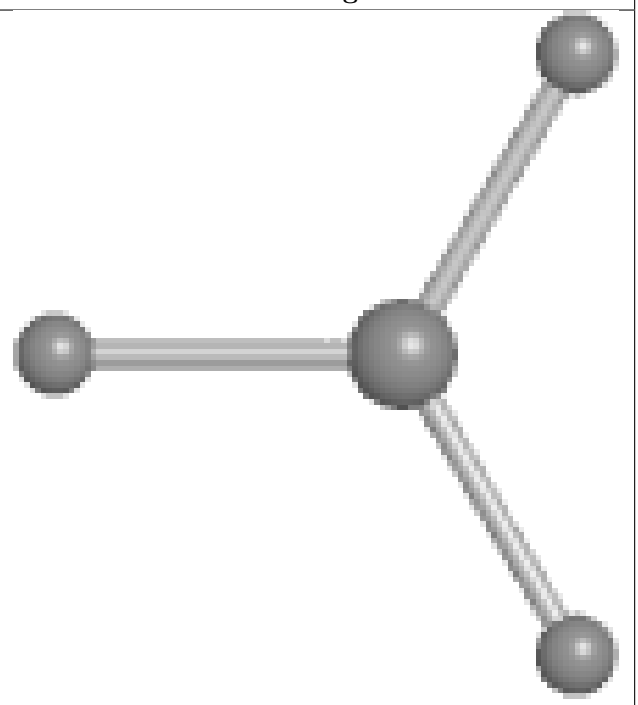
Bond lengths



Bond angles

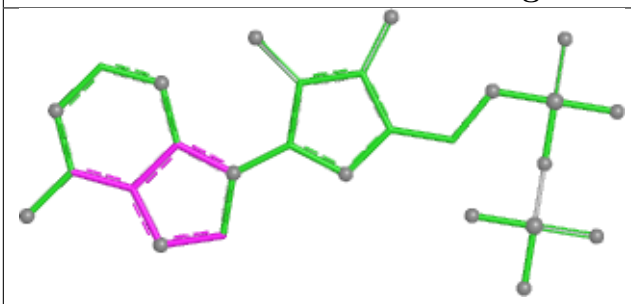


Torsions

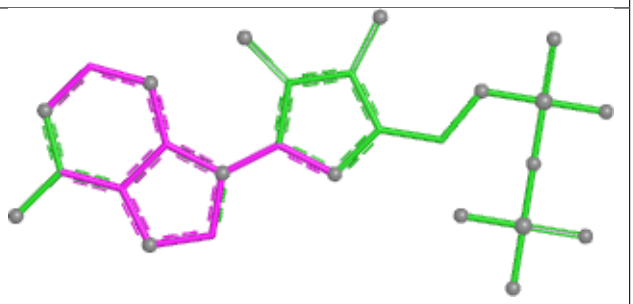


Rings

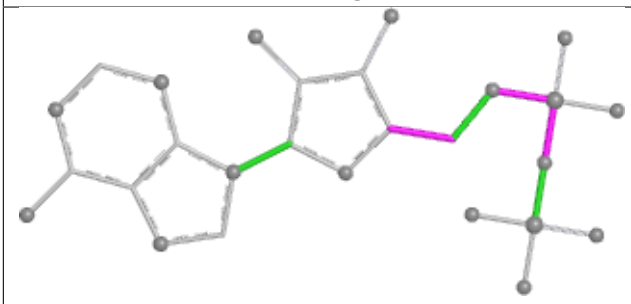
Ligand ADP B 602



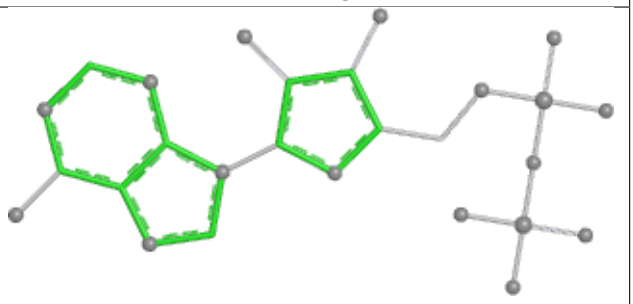
Bond lengths



Bond angles

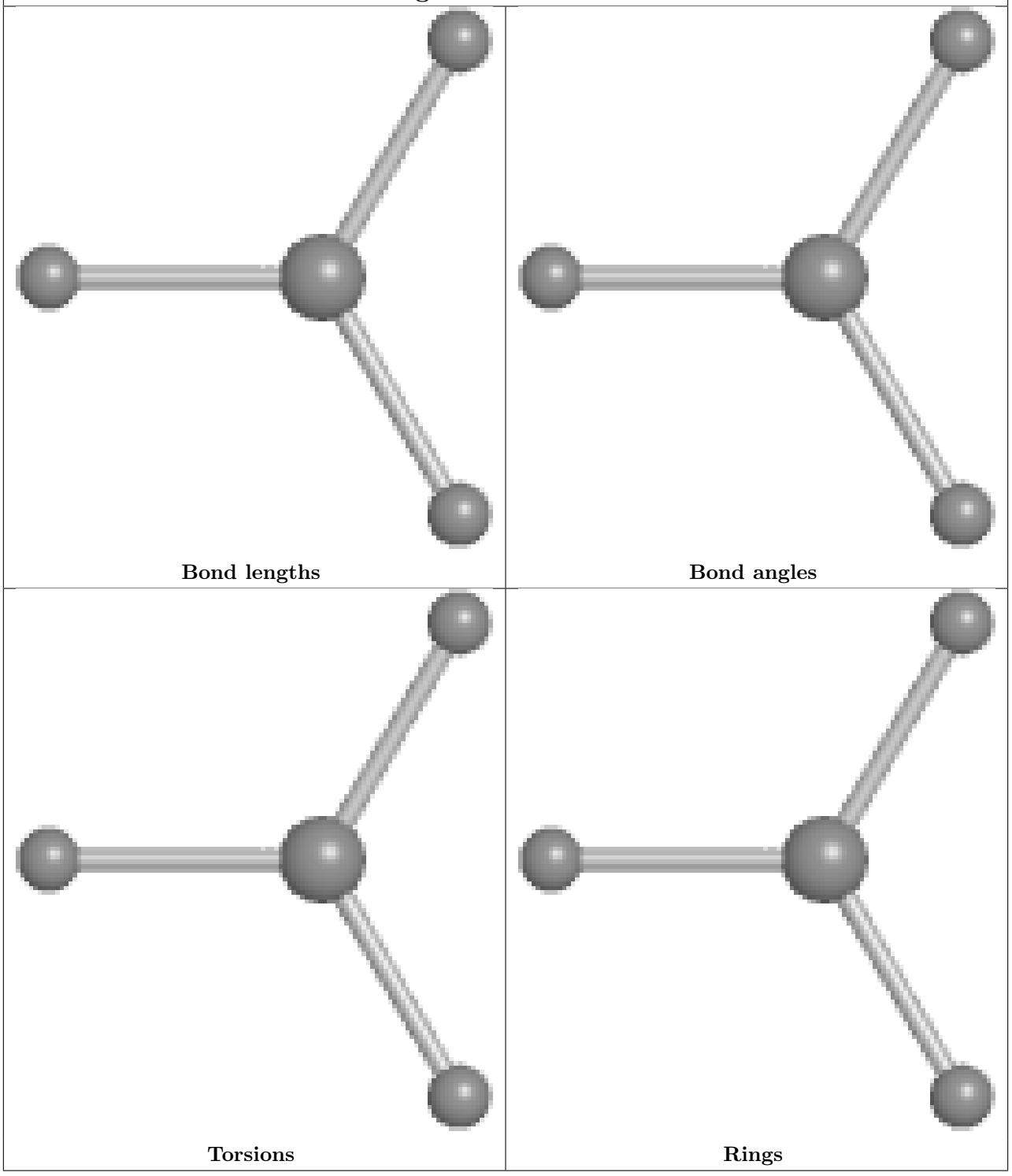


Torsions



Rings

Ligand AF3 G 603



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

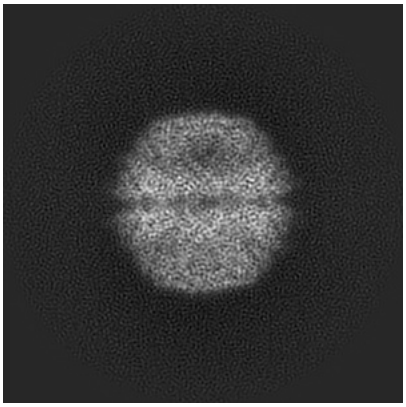
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-26123. These allow visual inspection of the internal detail of the map and identification of artifacts.

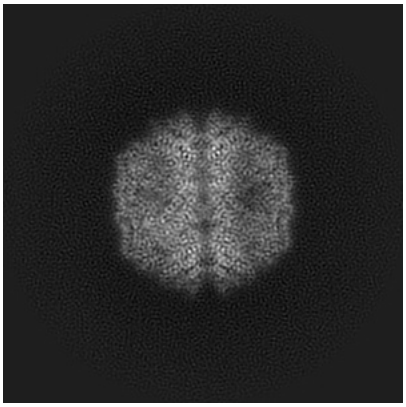
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

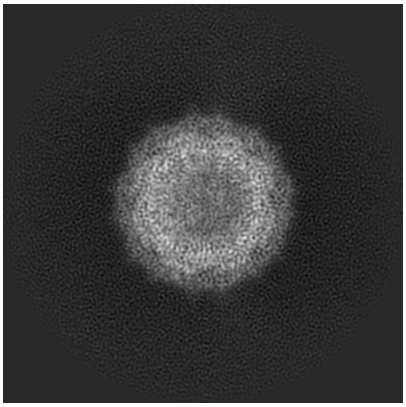
6.1.1 Primary map



X



Y

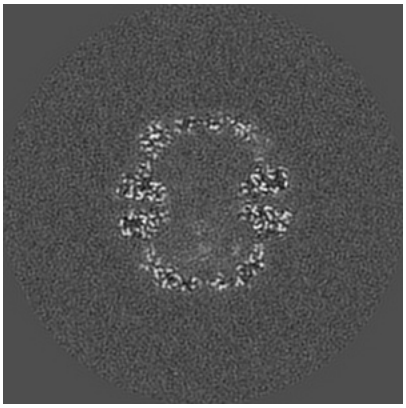


Z

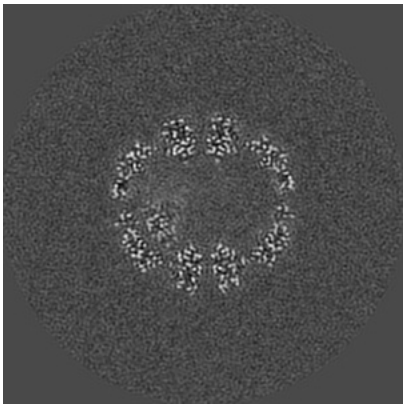
The images above show the map projected in three orthogonal directions.

6.2 Central slices

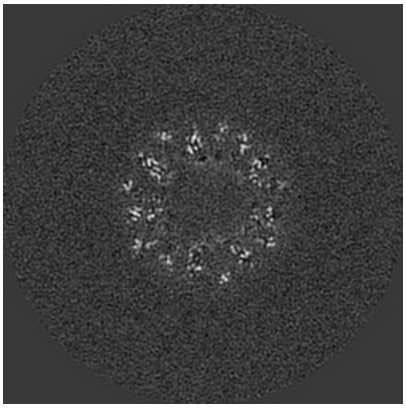
6.2.1 Primary map



X Index: 160



Y Index: 160

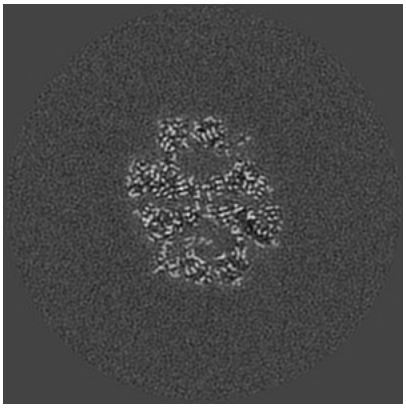


Z Index: 160

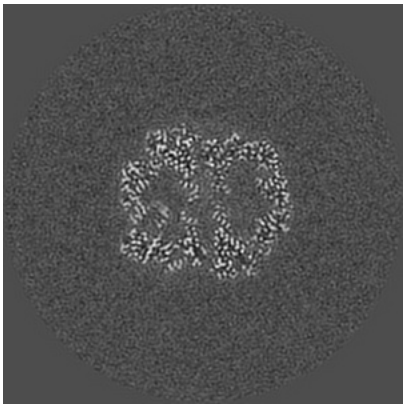
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

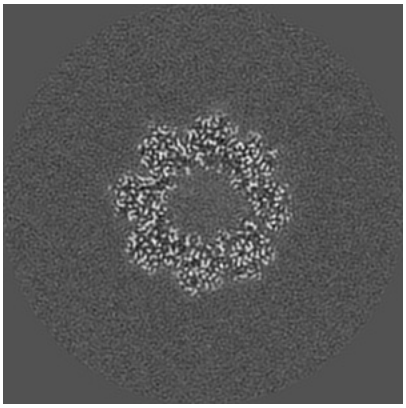
6.3.1 Primary map



X Index: 126



Y Index: 188

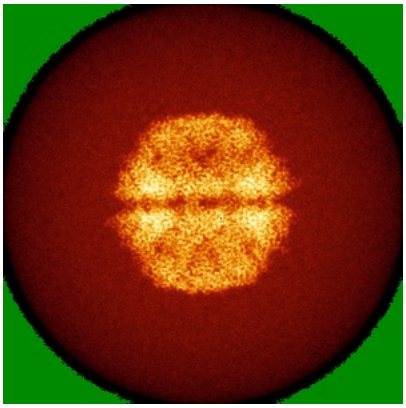


Z Index: 149

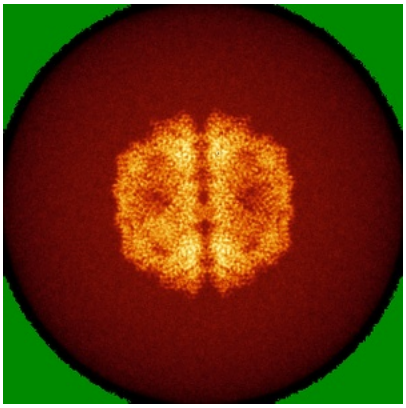
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

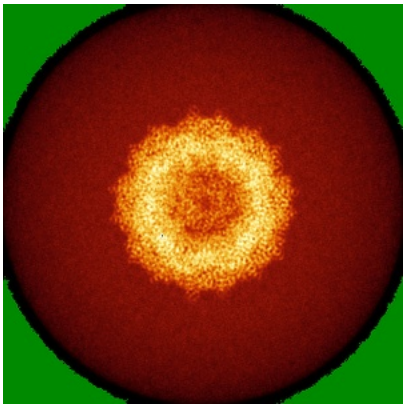
6.4.1 Primary map



X



Y

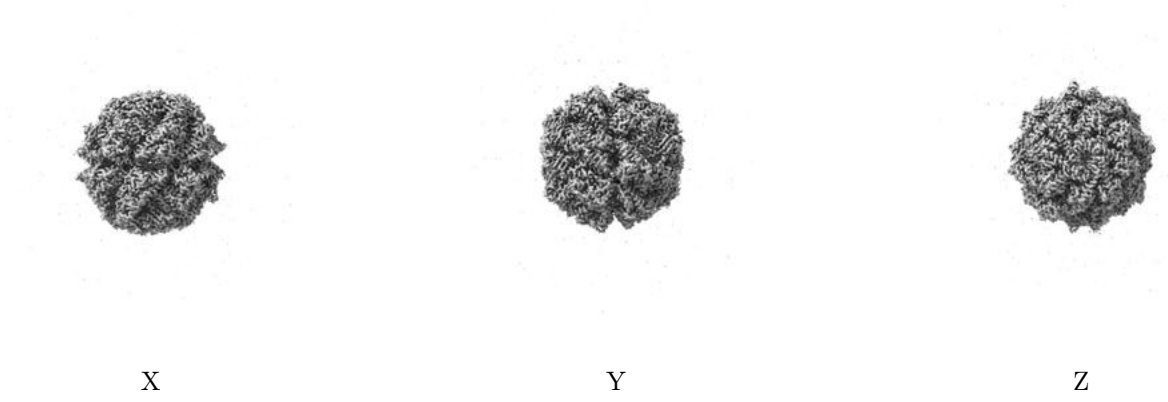


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.31. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

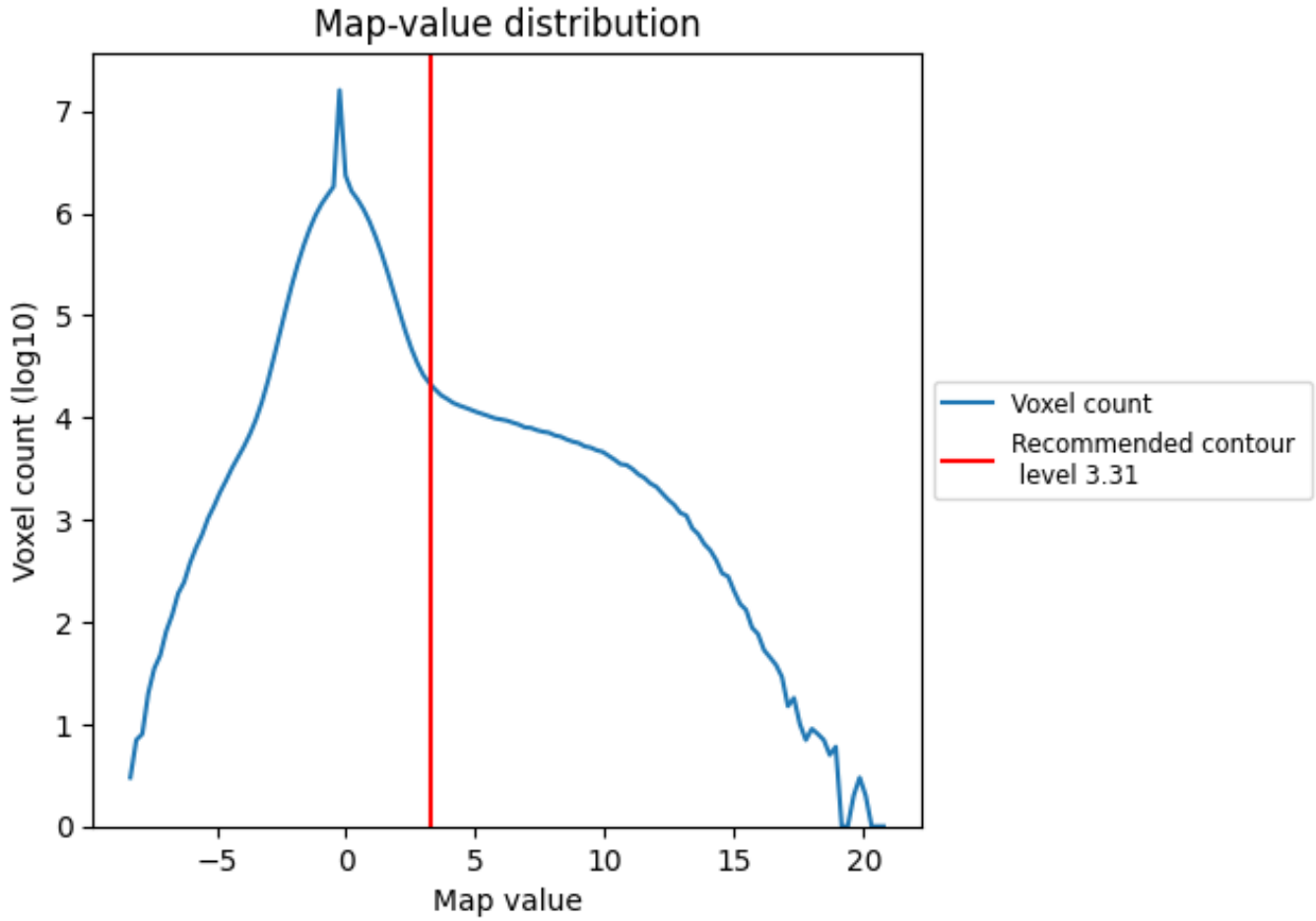
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

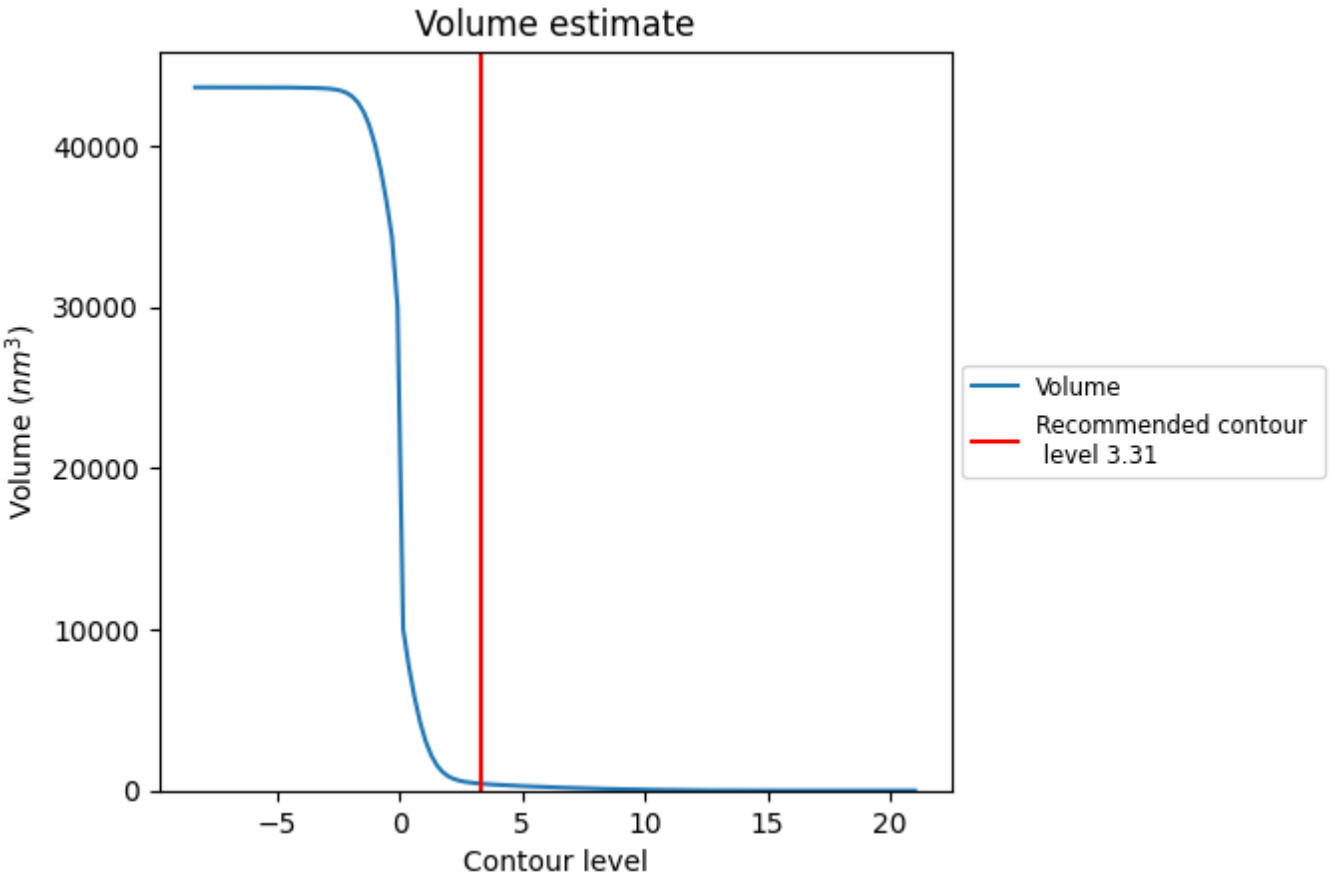
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

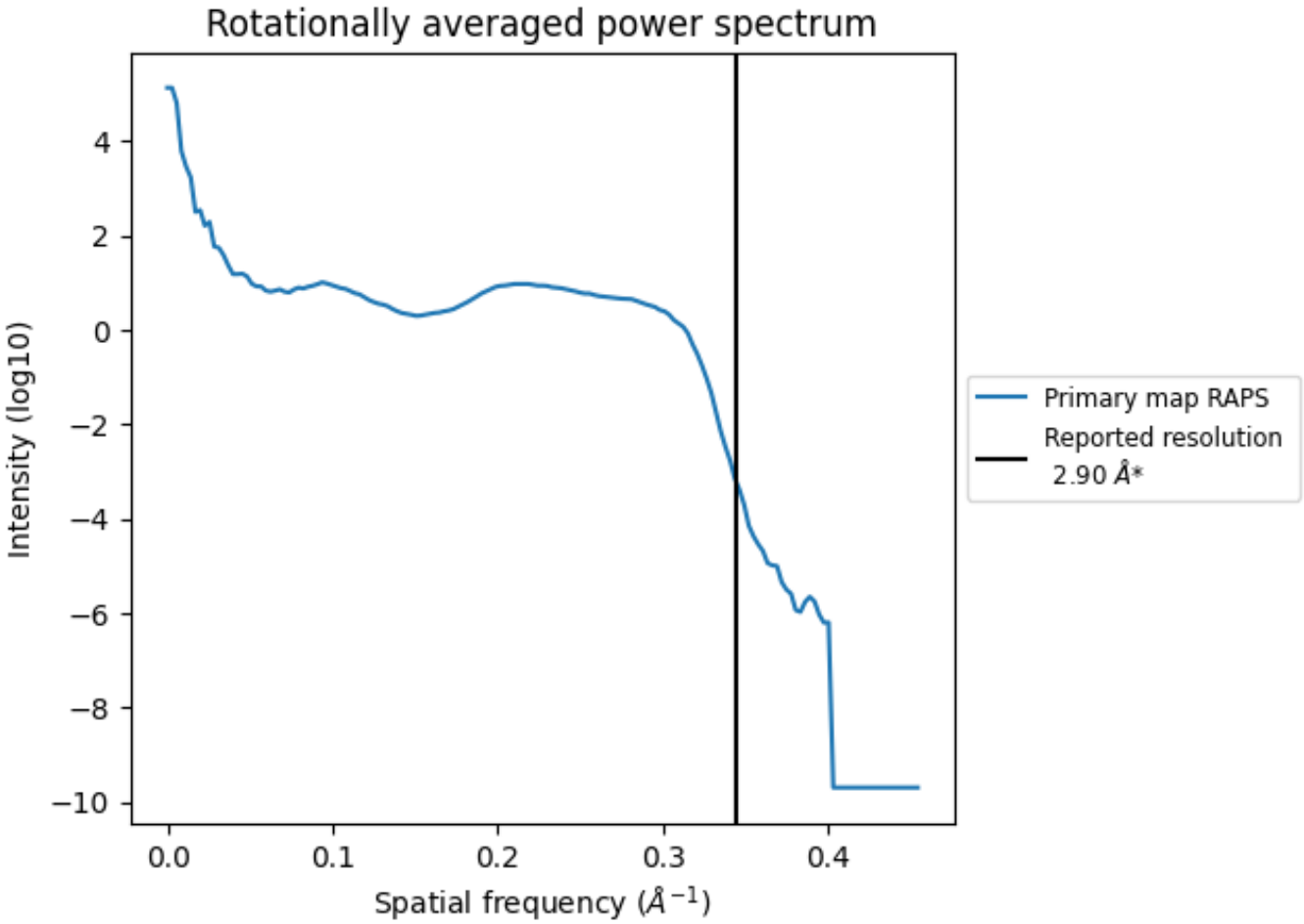
7.2 Volume estimate (i)



The volume at the recommended contour level is 428 nm^3; this corresponds to an approximate mass of 386 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

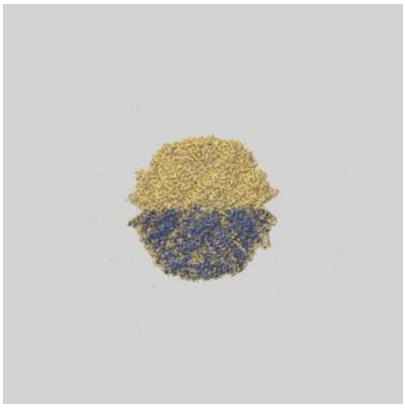
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

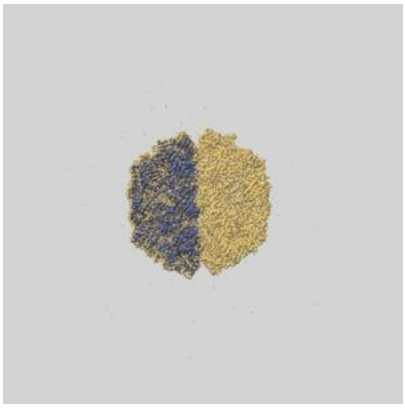
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-26123 and PDB model 7TTT. Per-residue inclusion information can be found in section 3 on page 9.

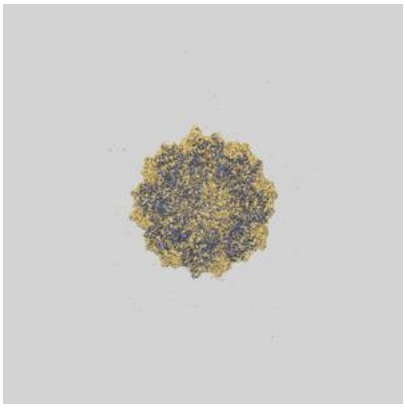
9.1 Map-model overlay



X



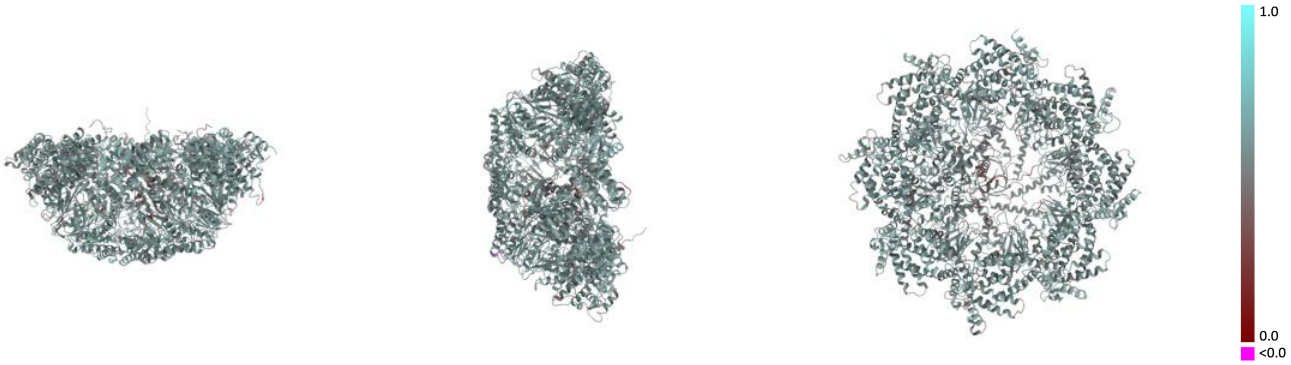
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.31 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

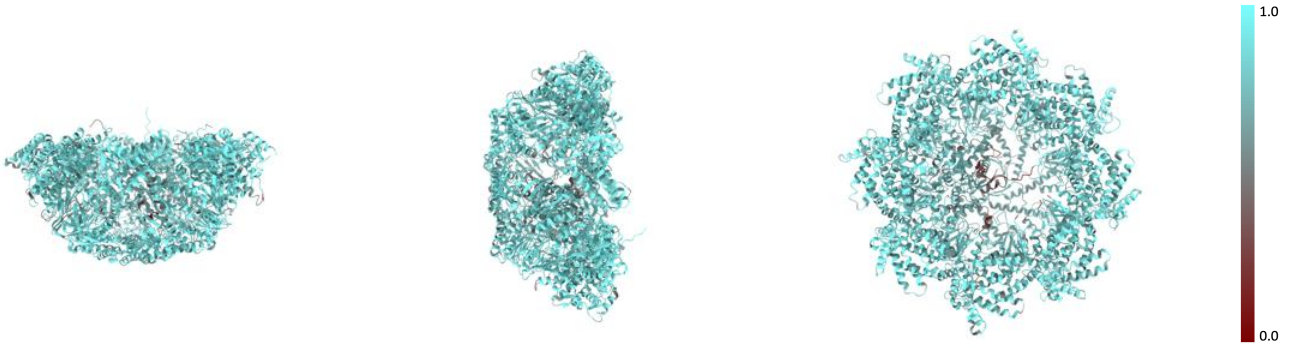
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

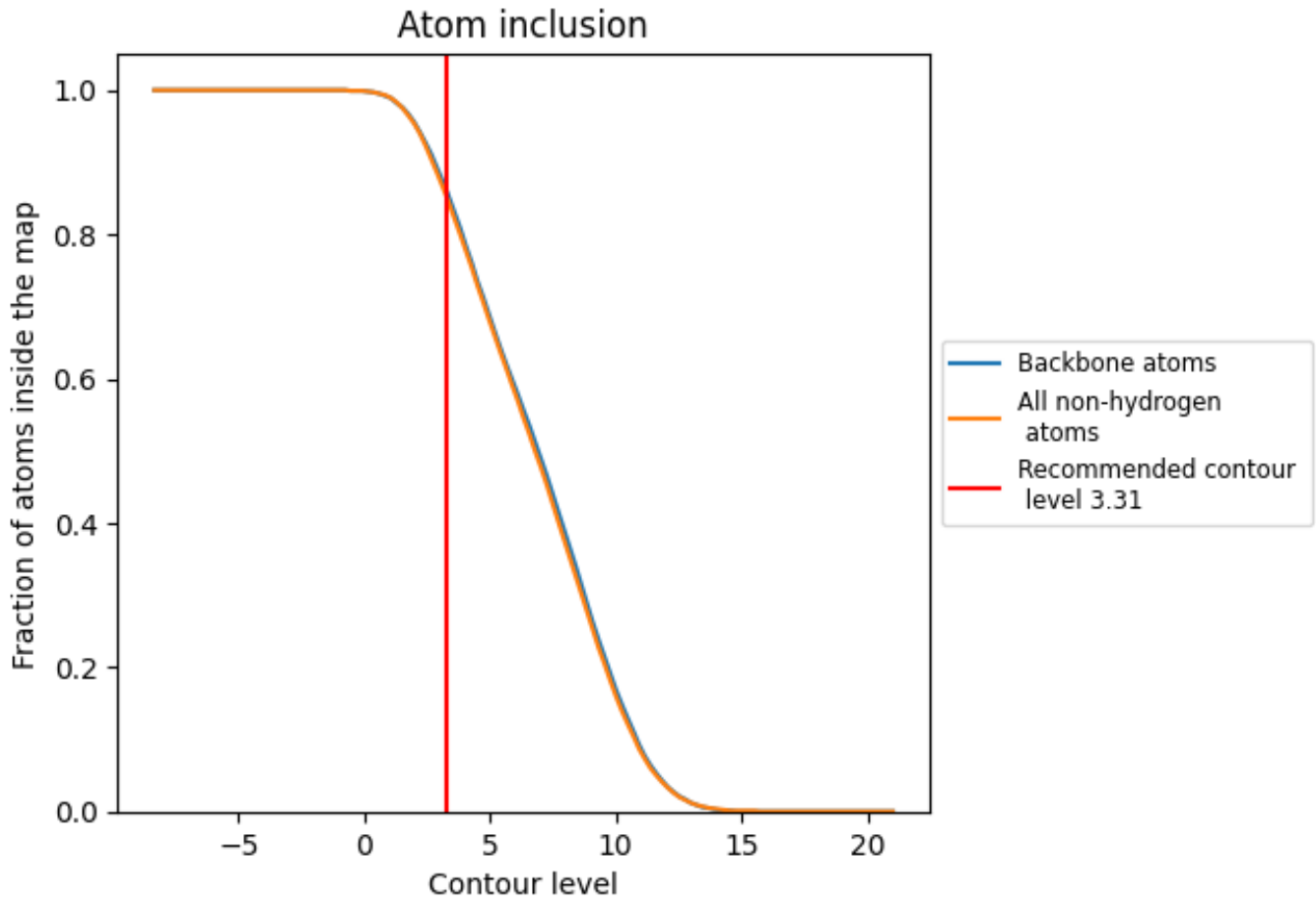
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.31).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.31) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5610
A	0.6860	0.5090
B	0.8650	0.5660
C	0.8780	0.5720
D	0.8630	0.5630
E	0.8640	0.5620
F	0.8550	0.5630
G	0.8560	0.5590
H	0.8750	0.5700
I	0.8680	0.5660

